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FIG. 1

| | | | | | | | | | | | | | | | | |
|--------|----|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SEQRES | 1 | A | 297 | MET | ALA | LEU | ALA | PRO | ASN | GLN | ALA | LEU | LEU | ARG | ILE | LEU |
| SEQRES | 2 | A | 297 | LYS | GLU | THR | GLU | PHE | LYS | LYS | ILE | LYS | VAL | LEU | GLY | SER |
| SEQRES | 3 | A | 297 | GLY | ALA | PHE | GLY | THR | VAL | TYR | LYS | GLY | LEU | TRP | ILE | PRO |
| SEQRES | 4 | A | 297 | GLU | GLY | GLU | LYS | VAL | LYS | ILE | PRO | VAL | ALA | ILE | LYS | GLU |
| SEQRES | 5 | A | 297 | LEU | ARG | GLU | ALA | THR | SER | PRO | LYS | ALA | ASN | LYS | GLU | ILE |
| SEQRES | 6 | A | 297 | LEU | ASP | GLU | ALA | TYR | VAL | MET | ALA | SER | VAL | ASP | ASN | PRO |
| SEQRES | 7 | A | 297 | HIS | VAL | CYS | ARG | LEU | LEU | GLY | ILE | CYS | LEU | THR | SER | THR |
| SEQRES | 8 | A | 297 | VAL | GLN | LEU | ILE | THR | GLN | LEU | MET | PRO | PHE | GLY | CYS | LEU |
| SEQRES | 9 | A | 297 | LEU | ASP | TYR | VAL | ARG | GLU | HIS | LYS | ASP | ASN | ILE | GLY | SER |
| SEQRES | 10 | A | 297 | GLN | TYR | LEU | LEU | ASN | TRP | CYS | VAL | GLN | ILE | ALA | LYS | GLY |
| SEQRES | 11 | A | 297 | MET | ASN | TYR | LEU | GLU | ASP | ARG | ARG | LEU | VAL | HIS | ARG | ASP |
| SEQRES | 12 | A | 297 | LEU | ALA | ALA | ARG | ASN | VAL | LEU | VAL | LYS | THR | PRO | GLN | HIS |
| SEQRES | 13 | A | 297 | VAL | LYS | ILE | THR | ASP | PHE | GLY | LEU | ALA | LYS | LEU | LEU | GLY |
| SEQRES | 14 | A | 297 | ALA | GLU | GLU | LYS | GLU | TYR | HIS | ALA | GLU | GLY | GLY | LYS | VAL |
| SEQRES | 15 | A | 297 | PRO | ILE | LYS | TRP | MET | ALA | LEU | GLU | SER | ILE | LEU | HIS | ARG |
| SEQRES | 16 | A | 297 | ILE | TYR | THR | HIS | GLN | SER | ASP | VAL | TRP | SER | TYR | GLY | VAL |
| SEQRES | 17 | A | 297 | THR | VAL | TRP | GLU | LEU | MET | THR | PHE | GLY | SER | LYS | PRO | TYR |
| SEQRES | 18 | A | 297 | ASP | GLY | ILE | PRO | ALA | SER | GLU | ILE | SER | SER | ILE | LEU | GLU |
| SEQRES | 19 | A | 297 | LYS | GLY | GLU | ARG | LEU | PRO | GLN | PRO | PRO | ILE | CYS | THR | ILE |
| SEQRES | 20 | A | 297 | ASP | VAL | TYR | MET | ILE | MET | VAL | LYS | CYS | TRP | MET | ILE | ASP |
| SEQRES | 21 | A | 297 | ALA | ASP | SER | ARG | PRO | LYS | PHE | ARG | GLU | LEU | ILE | ILE | GLU |
| SEQRES | 22 | A | 297 | PHE | SER | LYS | MET | ALA | ARG | ASP | PRO | GLN | ARG | TYR | LEU | VAL |
| SEQRES | 23 | A | 297 | ILE | GLN | GLY | GLU | GLY | HIS | HIS | HIS | HIS | HIS | HIS | HIS | |

FIG 2

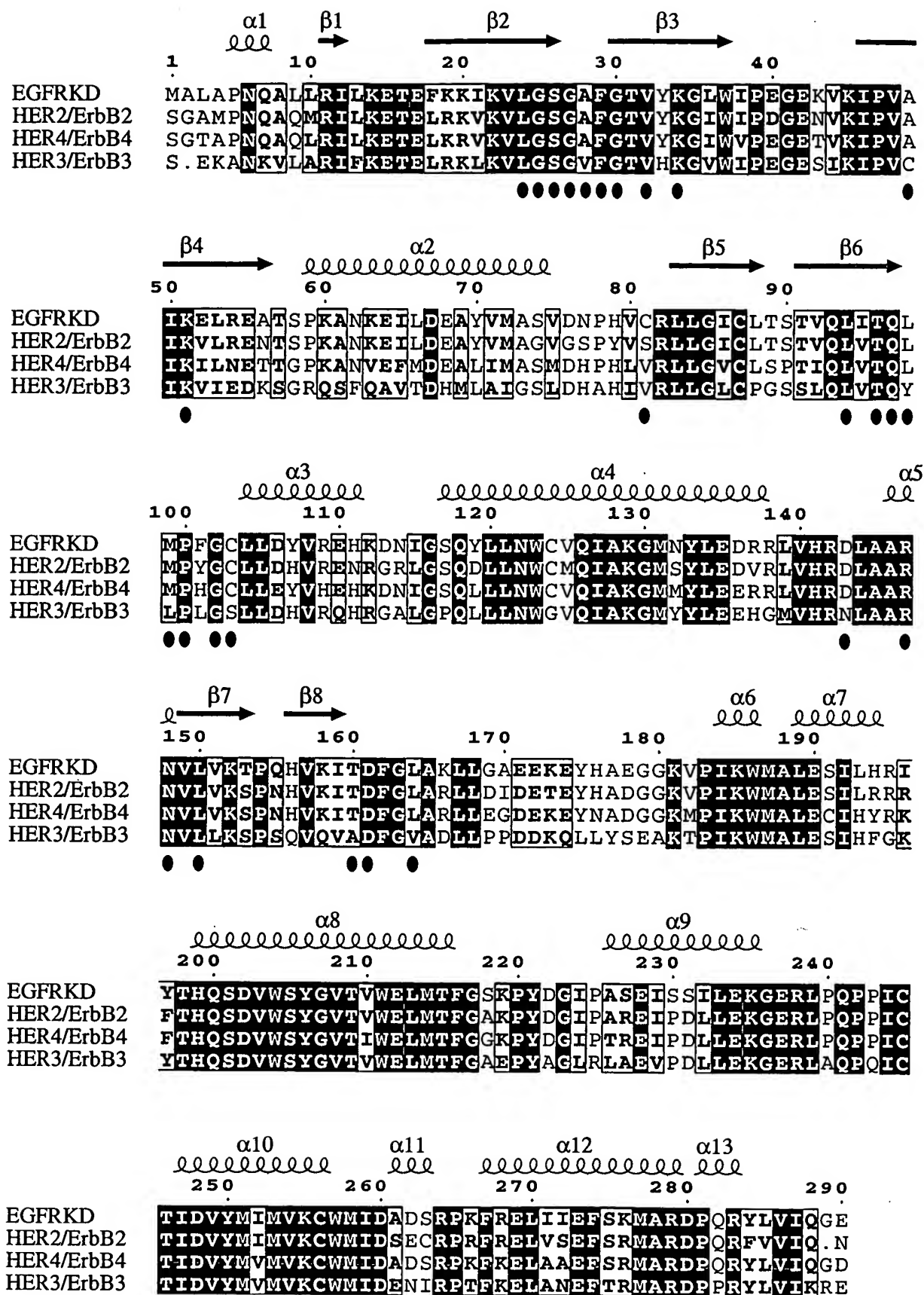


FIG. 3

CRYST1 56.926 64.948 80.249 90.00 109.01 90.00 P 1 21 1 2

| | Atom | | | | | | | | | |
|------|------|---------|-------|----|--------|---------|--------|------|-------|---|
| | Type | Residue | # | X | Y | Z | OCC | B | Atom | |
| ATOM | 1 | N | LEU A | 3 | 25.444 | -20.332 | 25.811 | 1.00 | 25.27 | N |
| ATOM | 2 | CA | LEU A | 3 | 26.210 | -21.613 | 25.815 | 1.00 | 25.21 | C |
| ATOM | 3 | C | LEU A | 3 | 27.671 | -21.412 | 25.400 | 1.00 | 25.54 | C |
| ATOM | 4 | O | LEU A | 3 | 28.579 | -21.944 | 26.039 | 1.00 | 25.74 | O |
| ATOM | 5 | CB | LEU A | 3 | 25.539 | -22.635 | 24.887 | 1.00 | 24.95 | C |
| ATOM | 6 | CG | LEU A | 3 | 24.252 | -23.372 | 25.286 | 1.00 | 24.41 | C |
| ATOM | 7 | CD1 | LEU A | 3 | 24.197 | -23.711 | 26.774 | 1.00 | 24.32 | C |
| ATOM | 8 | CD2 | LEU A | 3 | 23.016 | -22.583 | 24.867 | 1.00 | 24.49 | C |
| ATOM | 9 | N | ALA A | 4 | 27.881 | -20.636 | 24.337 | 1.00 | 25.85 | N |
| ATOM | 10 | CA | ALA A | 4 | 29.199 | -20.461 | 23.725 | 1.00 | 26.19 | C |
| ATOM | 11 | C | ALA A | 4 | 29.629 | -18.986 | 23.691 | 1.00 | 26.48 | C |
| ATOM | 12 | O | ALA A | 4 | 28.778 | -18.099 | 23.594 | 1.00 | 26.73 | O |
| ATOM | 13 | CB | ALA A | 4 | 29.194 | -21.050 | 22.318 | 1.00 | 26.08 | C |
| ATOM | 14 | N | PRO A | 5 | 30.938 | -18.723 | 23.767 | 1.00 | 26.64 | N |
| ATOM | 15 | CA | PRO A | 5 | 31.456 | -17.346 | 23.793 | 1.00 | 26.76 | C |
| ATOM | 16 | C | PRO A | 5 | 31.029 | -16.465 | 22.616 | 1.00 | 26.86 | C |
| ATOM | 17 | O | PRO A | 5 | 30.950 | -15.247 | 22.792 | 1.00 | 26.93 | O |
| ATOM | 18 | CB | PRO A | 5 | 32.980 | -17.536 | 23.797 | 1.00 | 26.73 | C |
| ATOM | 19 | CG | PRO A | 5 | 33.207 | -18.941 | 23.383 | 1.00 | 26.64 | C |
| ATOM | 20 | CD | PRO A | 5 | 32.025 | -19.714 | 23.861 | 1.00 | 26.62 | C |
| ATOM | 21 | N | ASN A | 6 | 30.754 | -17.058 | 21.455 | 1.00 | 27.05 | N |
| ATOM | 22 | CA | ASN A | 6 | 30.275 | -16.302 | 20.292 | 1.00 | 27.18 | C |
| ATOM | 23 | C | ASN A | 6 | 28.961 | -15.555 | 20.557 | 1.00 | 27.20 | C |
| ATOM | 24 | O | ASN A | 6 | 28.587 | -14.645 | 19.814 | 1.00 | 27.41 | O |
| ATOM | 25 | CB | ASN A | 6 | 30.147 | -17.208 | 19.059 | 1.00 | 27.19 | C |
| ATOM | 26 | CG | ASN A | 6 | 29.133 | -18.333 | 19.247 | 1.00 | 27.51 | C |
| ATOM | 27 | OD1 | ASN A | 6 | 28.433 | -18.402 | 20.258 | 1.00 | 28.16 | O |
| ATOM | 28 | ND2 | ASN A | 6 | 29.059 | -19.227 | 18.265 | 1.00 | 27.50 | N |
| ATOM | 29 | N | GLN A | 7 | 28.273 | -15.953 | 21.623 | 1.00 | 27.18 | N |
| ATOM | 30 | CA | GLN A | 7 | 27.037 | -15.310 | 22.054 | 1.00 | 27.07 | C |
| ATOM | 31 | C | GLN A | 7 | 27.309 | -14.181 | 23.056 | 1.00 | 26.85 | C |
| ATOM | 32 | O | GLN A | 7 | 26.374 | -13.599 | 23.612 | 1.00 | 26.95 | O |
| ATOM | 33 | CB | GLN A | 7 | 26.085 | -16.349 | 22.661 | 1.00 | 27.19 | C |
| ATOM | 34 | CG | GLN A | 7 | 25.571 | -17.396 | 21.672 | 1.00 | 27.57 | C |
| ATOM | 35 | CD | GLN A | 7 | 24.951 | -18.601 | 22.361 | 1.00 | 28.18 | C |
| ATOM | 36 | OE1 | GLN A | 7 | 25.663 | -19.453 | 22.899 | 1.00 | 28.63 | O |
| ATOM | 37 | NE2 | GLN A | 7 | 23.626 | -18.673 | 22.349 | 1.00 | 27.92 | N |
| ATOM | 38 | N | ALA A | 8 | 28.589 | -13.872 | 23.274 | 1.00 | 26.58 | N |
| ATOM | 39 | CA | ALA A | 8 | 28.996 | -12.883 | 24.272 | 1.00 | 26.34 | C |
| ATOM | 40 | C | ALA A | 8 | 30.309 | -12.153 | 23.943 | 1.00 | 26.18 | C |
| ATOM | 41 | O | ALA A | 8 | 30.800 | -11.358 | 24.750 | 1.00 | 26.16 | O |
| ATOM | 42 | CB | ALA A | 8 | 29.082 | -13.538 | 25.652 | 1.00 | 26.33 | C |
| ATOM | 43 | N | LEU A | 9 | 30.870 | -12.414 | 22.765 | 1.00 | 26.04 | N |
| ATOM | 44 | CA | LEU A | 9 | 32.142 | -11.805 | 22.372 | 1.00 | 25.90 | C |
| ATOM | 45 | C | LEU A | 9 | 31.969 | -10.684 | 21.351 | 1.00 | 25.81 | C |
| ATOM | 46 | O | LEU A | 9 | 31.094 | -10.743 | 20.486 | 1.00 | 25.85 | O |
| ATOM | 47 | CB | LEU A | 9 | 33.107 | -12.865 | 21.832 | 1.00 | 25.92 | C |
| ATOM | 48 | N | LEU A | 10 | 32.819 | -9.667 | 21.462 | 1.00 | 25.74 | N |
| ATOM | 49 | CA | LEU A | 10 | 32.791 | -8.520 | 20.562 | 1.00 | 25.61 | C |
| ATOM | 50 | C | LEU A | 10 | 33.690 | -8.744 | 19.354 | 1.00 | 25.72 | C |
| ATOM | 51 | O | LEU A | 10 | 34.847 | -9.145 | 19.492 | 1.00 | 25.75 | O |
| ATOM | 52 | CB | LEU A | 10 | 33.211 | -7.250 | 21.308 | 1.00 | 25.46 | C |
| ATOM | 53 | CG | LEU A | 10 | 33.315 | -5.936 | 20.529 | 1.00 | 25.17 | C |
| ATOM | 54 | CD1 | LEU A | 10 | 31.940 | -5.364 | 20.214 | 1.00 | 24.76 | C |
| ATOM | 55 | CD2 | LEU A | 10 | 34.153 | -4.937 | 21.312 | 1.00 | 25.05 | C |

FIG. 4A

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|--------|------|-------|---|
| ATOM | 56 | N | ARG | A | 11 | 33.148 | -8.478 | 18.170 | 1.00 | 25.94 | N |
| ATOM | 57 | CA | ARG | A | 11 | 33.905 | -8.617 | 16.936 | 1.00 | 26.20 | C |
| ATOM | 58 | C | ARG | A | 11 | 34.537 | -7.292 | 16.521 | 1.00 | 26.33 | C |
| ATOM | 59 | O | ARG | A | 11 | 33.848 | -6.284 | 16.358 | 1.00 | 26.36 | O |
| ATOM | 60 | CB | ARG | A | 11 | 33.018 | -9.173 | 15.821 | 1.00 | 26.25 | C |
| ATOM | 61 | CG | ARG | A | 11 | 33.630 | -10.347 | 15.080 | 1.00 | 26.65 | C |
| ATOM | 62 | CD | ARG | A | 11 | 33.347 | -11.708 | 15.706 | 1.00 | 26.95 | C |
| ATOM | 63 | NE | ARG | A | 11 | 32.289 | -12.422 | 14.993 | 1.00 | 27.57 | N |
| ATOM | 64 | CZ | ARG | A | 11 | 32.464 | -13.129 | 13.879 | 1.00 | 27.33 | C |
| ATOM | 65 | NH1 | ARG | A | 11 | 31.426 | -13.734 | 13.317 | 1.00 | 27.70 | N |
| ATOM | 66 | NH2 | ARG | A | 11 | 33.665 | -13.235 | 13.323 | 1.00 | 26.62 | N |
| ATOM | 67 | N | ILE | A | 12 | 35.859 | -7.301 | 16.378 | 1.00 | 26.56 | N |
| ATOM | 68 | CA | ILE | A | 12 | 36.595 | -6.136 | 15.905 | 1.00 | 26.77 | C |
| ATOM | 69 | C | ILE | A | 12 | 36.489 | -6.113 | 14.391 | 1.00 | 26.96 | C |
| ATOM | 70 | O | ILE | A | 12 | 36.950 | -7.038 | 13.718 | 1.00 | 27.20 | O |
| ATOM | 71 | N | LEU | A | 13 | 35.873 | -5.063 | 13.860 | 1.00 | 27.07 | N |
| ATOM | 72 | CA | LEU | A | 13 | 35.599 | -4.989 | 12.431 | 1.00 | 27.24 | C |
| ATOM | 73 | C | LEU | A | 13 | 36.569 | -4.077 | 11.689 | 1.00 | 27.51 | C |
| ATOM | 74 | O | LEU | A | 13 | 36.891 | -2.980 | 12.157 | 1.00 | 27.50 | O |
| ATOM | 75 | CB | LEU | A | 13 | 34.152 | -4.543 | 12.183 | 1.00 | 27.16 | C |
| ATOM | 76 | CG | LEU | A | 13 | 32.963 | -5.509 | 12.340 | 1.00 | 27.13 | C |
| ATOM | 77 | CD1 | LEU | A | 13 | 32.136 | -5.548 | 11.062 | 1.00 | 26.77 | C |
| ATOM | 78 | CD2 | LEU | A | 13 | 33.355 | -6.927 | 12.757 | 1.00 | 27.33 | C |
| ATOM | 79 | N | LYS | A | 14 | 37.042 | -4.552 | 10.538 | 1.00 | 27.82 | N |
| ATOM | 80 | CA | LYS | A | 14 | 37.758 | -3.715 | 9.578 | 1.00 | 28.13 | C |
| ATOM | 81 | C | LYS | A | 14 | 36.718 | -3.087 | 8.666 | 1.00 | 28.13 | C |
| ATOM | 82 | O | LYS | A | 14 | 35.707 | -3.715 | 8.352 | 1.00 | 28.15 | O |
| ATOM | 83 | CB | LYS | A | 14 | 38.739 | -4.542 | 8.745 | 1.00 | 28.25 | C |
| ATOM | 84 | CG | LYS | A | 14 | 39.971 | -5.023 | 9.497 | 1.00 | 28.61 | C |
| ATOM | 85 | CD | LYS | A | 14 | 40.331 | -6.444 | 9.089 | 1.00 | 29.24 | C |
| ATOM | 86 | CE | LYS | A | 14 | 41.812 | -6.577 | 8.759 | 1.00 | 29.63 | C |
| ATOM | 87 | NZ | LYS | A | 14 | 42.548 | -7.356 | 9.800 | 1.00 | 29.62 | N |
| ATOM | 88 | N | GLU | A | 15 | 36.965 | -1.854 | 8.233 | 1.00 | 28.25 | N |
| ATOM | 89 | CA | GLU | A | 15 | 35.994 | -1.128 | 7.415 | 1.00 | 28.46 | C |
| ATOM | 90 | C | GLU | A | 15 | 35.778 | -1.719 | 6.009 | 1.00 | 28.36 | C |
| ATOM | 91 | O | GLU | A | 15 | 34.960 | -1.212 | 5.239 | 1.00 | 28.40 | O |
| ATOM | 92 | CB | GLU | A | 15 | 36.304 | 0.378 | 7.383 | 1.00 | 28.64 | C |
| ATOM | 93 | CG | GLU | A | 15 | 37.457 | 0.806 | 6.489 | 1.00 | 29.59 | C |
| ATOM | 94 | CD | GLU | A | 15 | 37.431 | 2.296 | 6.181 | 1.00 | 30.53 | C |
| ATOM | 95 | OE1 | GLU | A | 15 | 37.154 | 3.102 | 7.100 | 1.00 | 30.46 | O |
| ATOM | 96 | OE2 | GLU | A | 15 | 37.688 | 2.667 | 5.015 | 1.00 | 31.29 | O |
| ATOM | 97 | N | THR | A | 16 | 36.501 | -2.794 | 5.696 | 1.00 | 28.25 | N |
| ATOM | 98 | CA | THR | A | 16 | 36.305 | -3.536 | 4.449 | 1.00 | 28.09 | C |
| ATOM | 99 | C | THR | A | 16 | 35.501 | -4.819 | 4.680 | 1.00 | 27.97 | C |
| ATOM | 100 | O | THR | A | 16 | 35.098 | -5.490 | 3.725 | 1.00 | 27.77 | O |
| ATOM | 101 | CB | THR | A | 16 | 37.655 | -3.871 | 3.774 | 1.00 | 28.10 | C |
| ATOM | 102 | OG1 | THR | A | 16 | 38.469 | -4.632 | 4.675 | 1.00 | 28.22 | O |
| ATOM | 103 | CG2 | THR | A | 16 | 38.472 | -2.607 | 3.520 | 1.00 | 28.14 | C |
| ATOM | 104 | N | GLU | A | 17 | 35.273 | -5.151 | 5.949 | 1.00 | 27.87 | N |
| ATOM | 105 | CA | GLU | A | 17 | 34.484 | -6.326 | 6.319 | 1.00 | 27.81 | C |
| ATOM | 106 | C | GLU | A | 17 | 32.975 | -6.059 | 6.306 | 1.00 | 27.66 | C |
| ATOM | 107 | O | GLU | A | 17 | 32.177 | -6.995 | 6.358 | 1.00 | 27.72 | O |
| ATOM | 108 | CB | GLU | A | 17 | 34.919 | -6.861 | 7.687 | 1.00 | 27.91 | C |
| ATOM | 109 | CG | GLU | A | 17 | 36.190 | -7.695 | 7.647 | 1.00 | 28.09 | C |
| ATOM | 110 | CD | GLU | A | 17 | 36.659 | -8.119 | 9.025 | 1.00 | 28.50 | C |
| ATOM | 111 | OE1 | GLU | A | 17 | 37.107 | -7.246 | 9.797 | 1.00 | 28.53 | O |
| ATOM | 112 | OE2 | GLU | A | 17 | 36.586 | -9.328 | 9.336 | 1.00 | 28.89 | O |
| ATOM | 113 | N | PHE | A | 18 | 32.589 | -4.786 | 6.236 | 1.00 | 27.51 | N |
| ATOM | 114 | CA | PHE | A | 18 | 31.176 | -4.407 | 6.185 | 1.00 | 27.26 | C |
| ATOM | 115 | C | PHE | A | 18 | 30.905 | -3.280 | 5.191 | 1.00 | 27.26 | C |

FIG. 4B

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 116 | O | PHE | A | 18 | 31.786 | -2.468 | 4.898 | 1.00 | 27.35 | O |
| ATOM | 117 | CB | PHE | A | 18 | 30.652 | -4.039 | 7.583 | 1.00 | 27.13 | C |
| ATOM | 118 | CG | PHE | A | 18 | 31.166 | -2.724 | 8.107 | 1.00 | 26.95 | C |
| ATOM | 119 | CD1 | PHE | A | 18 | 30.396 | -1.569 | 8.003 | 1.00 | 26.76 | C |
| ATOM | 120 | CE1 | PHE | A | 18 | 30.866 | -0.350 | 8.488 | 1.00 | 26.83 | C |
| ATOM | 121 | CZ | PHE | A | 18 | 32.118 | -0.280 | 9.090 | 1.00 | 26.83 | C |
| ATOM | 122 | CE2 | PHE | A | 18 | 32.893 | -1.429 | 9.203 | 1.00 | 26.91 | C |
| ATOM | 123 | CD2 | PHE | A | 18 | 32.415 | -2.642 | 8.717 | 1.00 | 26.86 | C |
| ATOM | 124 | N | LYS | A | 19 | 29.673 | -3.241 | 4.686 | 1.00 | 27.10 | N |
| ATOM | 125 | CA | LYS | A | 19 | 29.239 | -2.217 | 3.744 | 1.00 | 26.92 | C |
| ATOM | 126 | C | LYS | A | 19 | 27.835 | -1.714 | 4.089 | 1.00 | 26.82 | C |
| ATOM | 127 | O | LYS | A | 19 | 26.937 | -2.511 | 4.380 | 1.00 | 26.80 | O |
| ATOM | 128 | CB | LYS | A | 19 | 29.271 | -2.769 | 2.316 | 1.00 | 26.91 | C |
| ATOM | 129 | CG | LYS | A | 19 | 29.342 | -1.706 | 1.232 | 1.00 | 27.23 | C |
| ATOM | 130 | N | LYS | A | 20 | 27.662 | -0.393 | 4.059 | 1.00 | 26.60 | N |
| ATOM | 131 | CA | LYS | A | 20 | 26.364 | 0.240 | 4.291 | 1.00 | 26.42 | C |
| ATOM | 132 | C | LYS | A | 20 | 25.620 | 0.389 | 2.969 | 1.00 | 26.34 | C |
| ATOM | 133 | O | LYS | A | 20 | 26.113 | 1.040 | 2.045 | 1.00 | 26.28 | O |
| ATOM | 134 | CB | LYS | A | 20 | 26.533 | 1.616 | 4.947 | 1.00 | 26.39 | C |
| ATOM | 135 | CG | LYS | A | 20 | 27.216 | 1.596 | 6.311 | 1.00 | 26.56 | C |
| ATOM | 136 | CD | LYS | A | 20 | 27.464 | 3.005 | 6.844 | 1.00 | 26.29 | C |
| ATOM | 137 | CE | LYS | A | 20 | 28.684 | 3.660 | 6.206 | 1.00 | 26.38 | C |
| ATOM | 138 | NZ | LYS | A | 20 | 29.963 | 3.012 | 6.612 | 1.00 | 26.50 | N |
| ATOM | 139 | N | ILE | A | 21 | 24.436 | -0.215 | 2.881 | 1.00 | 26.31 | N |
| ATOM | 140 | CA | ILE | A | 21 | 23.650 | -0.180 | 1.649 | 1.00 | 26.28 | C |
| ATOM | 141 | C | ILE | A | 21 | 22.658 | 0.987 | 1.624 | 1.00 | 26.44 | C |
| ATOM | 142 | O | ILE | A | 21 | 22.652 | 1.763 | 0.673 | 1.00 | 26.65 | O |
| ATOM | 143 | CB | ILE | A | 21 | 22.970 | -1.552 | 1.368 | 1.00 | 26.22 | C |
| ATOM | 144 | CG1 | ILE | A | 21 | 24.001 | -2.556 | 0.857 | 1.00 | 26.16 | C |
| ATOM | 145 | CD1 | ILE | A | 21 | 24.390 | -3.591 | 1.868 | 1.00 | 26.80 | C |
| ATOM | 146 | CG2 | ILE | A | 21 | 21.860 | -1.428 | 0.332 | 1.00 | 26.00 | C |
| ATOM | 147 | N | LYS | A | 22 | 21.832 | 1.116 | 2.661 | 1.00 | 26.52 | N |
| ATOM | 148 | CA | LYS | A | 22 | 20.870 | 2.219 | 2.724 | 1.00 | 26.71 | C |
| ATOM | 149 | C | LYS | A | 22 | 20.505 | 2.636 | 4.149 | 1.00 | 26.80 | C |
| ATOM | 150 | O | LYS | A | 22 | 20.413 | 1.801 | 5.051 | 1.00 | 26.76 | O |
| ATOM | 151 | CB | LYS | A | 22 | 19.607 | 1.910 | 1.906 | 1.00 | 26.76 | C |
| ATOM | 152 | CG | LYS | A | 22 | 18.932 | 0.587 | 2.232 | 1.00 | 27.25 | C |
| ATOM | 153 | CD | LYS | A | 22 | 17.460 | 0.785 | 2.544 | 1.00 | 27.75 | C |
| ATOM | 154 | CE | LYS | A | 22 | 16.585 | 0.496 | 1.331 | 1.00 | 27.67 | C |
| ATOM | 155 | NZ | LYS | A | 22 | 16.435 | 1.690 | 0.455 | 1.00 | 27.22 | N |
| ATOM | 156 | N | VAL | A | 23 | 20.298 | 3.939 | 4.327 | 1.00 | 26.71 | N |
| ATOM | 157 | CA | VAL | A | 23 | 19.968 | 4.522 | 5.625 | 1.00 | 26.86 | C |
| ATOM | 158 | C | VAL | A | 23 | 18.538 | 4.178 | 6.056 | 1.00 | 26.96 | C |
| ATOM | 159 | O | VAL | A | 23 | 17.597 | 4.294 | 5.269 | 1.00 | 27.12 | O |
| ATOM | 160 | CB | VAL | A | 23 | 20.220 | 6.073 | 5.640 | 1.00 | 26.92 | C |
| ATOM | 161 | CG1 | VAL | A | 23 | 19.866 | 6.713 | 4.304 | 1.00 | 27.07 | C |
| ATOM | 162 | CG2 | VAL | A | 23 | 19.469 | 6.764 | 6.774 | 1.00 | 26.77 | C |
| ATOM | 163 | N | LEU | A | 24 | 18.401 | 3.732 | 7.304 | 1.00 | 27.04 | N |
| ATOM | 164 | CA | LEU | A | 24 | 17.104 | 3.474 | 7.924 | 1.00 | 27.04 | C |
| ATOM | 165 | C | LEU | A | 24 | 16.553 | 4.752 | 8.548 | 1.00 | 27.12 | C |
| ATOM | 166 | O | LEU | A | 24 | 15.349 | 5.011 | 8.506 | 1.00 | 27.14 | O |
| ATOM | 167 | CB | LEU | A | 24 | 17.244 | 2.415 | 9.020 | 1.00 | 27.15 | C |
| ATOM | 168 | CG | LEU | A | 24 | 16.966 | 0.944 | 8.719 | 1.00 | 27.16 | C |
| ATOM | 169 | CD1 | LEU | A | 24 | 17.690 | 0.080 | 9.737 | 1.00 | 27.29 | C |
| ATOM | 170 | CD2 | LEU | A | 24 | 15.474 | 0.649 | 8.743 | 1.00 | 27.56 | C |
| ATOM | 171 | N | GLY | A | 25 | 17.449 | 5.539 | 9.139 | 1.00 | 27.10 | N |
| ATOM | 172 | CA | GLY | A | 25 | 17.078 | 6.762 | 9.821 | 1.00 | 27.12 | C |
| ATOM | 173 | C | GLY | A | 25 | 18.140 | 7.230 | 10.799 | 1.00 | 27.13 | C |
| ATOM | 174 | O | GLY | A | 25 | 19.211 | 6.632 | 10.911 | 1.00 | 27.18 | O |
| ATOM | 175 | N | SER | A | 26 | 17.831 | 8.309 | 11.508 | 1.00 | 27.13 | N |

FIG. 4C

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 176 | CA | SER | A | 26 | 18.771 | 8.926 | 12.432 | 1.00 | 27.27 | C |
| ATOM | 177 | C | SER | A | 26 | 18.074 | 9.331 | 13.726 | 1.00 | 27.18 | C |
| ATOM | 178 | O | SER | A | 26 | 16.884 | 9.660 | 13.726 | 1.00 | 27.29 | O |
| ATOM | 179 | CB | SER | A | 26 | 19.442 | 10.139 | 11.778 | 1.00 | 27.33 | C |
| ATOM | 180 | OG | SER | A | 26 | 18.724 | 11.335 | 12.040 | 1.00 | 27.76 | O |
| ATOM | 181 | N | GLY | A | 27 | 18.825 | 9.303 | 14.823 | 1.00 | 26.97 | N |
| ATOM | 182 | CA | GLY | A | 27 | 18.303 | 9.683 | 16.123 | 1.00 | 26.91 | C |
| ATOM | 183 | C | GLY | A | 27 | 19.148 | 10.749 | 16.785 | 1.00 | 26.84 | C |
| ATOM | 184 | O | GLY | A | 27 | 19.693 | 11.626 | 16.112 | 1.00 | 26.96 | O |
| ATOM | 185 | N | ALA | A | 28 | 19.260 | 10.663 | 18.108 | 1.00 | 26.71 | N |
| ATOM | 186 | CA | ALA | A | 28 | 19.994 | 11.652 | 18.895 | 1.00 | 26.48 | C |
| ATOM | 187 | C | ALA | A | 28 | 21.434 | 11.224 | 19.191 | 1.00 | 26.40 | C |
| ATOM | 188 | O | ALA | A | 28 | 22.094 | 11.805 | 20.054 | 1.00 | 26.77 | O |
| ATOM | 189 | CB | ALA | A | 28 | 19.247 | 11.952 | 20.186 | 1.00 | 26.32 | C |
| ATOM | 190 | N | PHE | A | 29 | 21.917 | 10.205 | 18.484 | 1.00 | 25.95 | N |
| ATOM | 191 | CA | PHE | A | 29 | 23.289 | 9.735 | 18.664 | 1.00 | 25.62 | C |
| ATOM | 192 | C | PHE | A | 29 | 24.001 | 9.495 | 17.334 | 1.00 | 25.26 | C |
| ATOM | 193 | O | PHE | A | 29 | 25.229 | 9.555 | 17.266 | 1.00 | 25.24 | O |
| ATOM | 194 | CB | PHE | A | 29 | 23.329 | 8.472 | 19.531 | 1.00 | 25.74 | C |
| ATOM | 195 | CG | PHE | A | 29 | 22.739 | 8.656 | 20.907 | 1.00 | 26.20 | C |
| ATOM | 196 | CD1 | PHE | A | 29 | 21.499 | 8.106 | 21.225 | 1.00 | 26.43 | C |
| ATOM | 197 | CE1 | PHE | A | 29 | 20.947 | 8.275 | 22.499 | 1.00 | 26.45 | C |
| ATOM | 198 | CZ | PHE | A | 29 | 21.638 | 8.999 | 23.466 | 1.00 | 26.14 | C |
| ATOM | 199 | CE2 | PHE | A | 29 | 22.875 | 9.553 | 23.159 | 1.00 | 26.30 | C |
| ATOM | 200 | CD2 | PHE | A | 29 | 23.421 | 9.378 | 21.885 | 1.00 | 26.38 | C |
| ATOM | 201 | N | GLY | A | 30 | 23.231 | 9.231 | 16.281 | 1.00 | 24.84 | N |
| ATOM | 202 | CA | GLY | A | 30 | 23.798 | 8.993 | 14.967 | 1.00 | 24.15 | C |
| ATOM | 203 | C | GLY | A | 30 | 22.830 | 8.427 | 13.948 | 1.00 | 23.71 | C |
| ATOM | 204 | O | GLY | A | 30 | 21.634 | 8.305 | 14.209 | 1.00 | 23.87 | O |
| ATOM | 205 | N | THR | A | 31 | 23.364 | 8.086 | 12.778 | 1.00 | 23.20 | N |
| ATOM | 206 | CA | THR | A | 31 | 22.581 | 7.536 | 11.679 | 1.00 | 22.50 | C |
| ATOM | 207 | C | THR | A | 31 | 22.704 | 6.013 | 11.640 | 1.00 | 22.16 | C |
| ATOM | 208 | O | THR | A | 31 | 23.792 | 5.463 | 11.821 | 1.00 | 21.56 | O |
| ATOM | 209 | CB | THR | A | 31 | 23.042 | 8.159 | 10.339 | 1.00 | 22.68 | C |
| ATOM | 210 | OG1 | THR | A | 31 | 22.930 | 9.587 | 10.412 | 1.00 | 22.50 | O |
| ATOM | 211 | CG2 | THR | A | 31 | 22.096 | 7.792 | 9.200 | 1.00 | 22.19 | C |
| ATOM | 212 | N | VAL | A | 32 | 21.573 | 5.346 | 11.414 | 1.00 | 21.96 | N |
| ATOM | 213 | CA | VAL | A | 32 | 21.526 | 3.890 | 11.300 | 1.00 | 21.83 | C |
| ATOM | 214 | C | VAL | A | 32 | 21.336 | 3.490 | 9.840 | 1.00 | 21.81 | C |
| ATOM | 215 | O | VAL | A | 32 | 20.497 | 4.054 | 9.133 | 1.00 | 21.57 | O |
| ATOM | 216 | CB | VAL | A | 32 | 20.397 | 3.264 | 12.168 | 1.00 | 21.85 | C |
| ATOM | 217 | CG1 | VAL | A | 32 | 20.461 | 1.737 | 12.134 | 1.00 | 21.60 | C |
| ATOM | 218 | CG2 | VAL | A | 32 | 20.472 | 3.763 | 13.603 | 1.00 | 21.69 | C |
| ATOM | 219 | N | TYR | A | 33 | 22.127 | 2.512 | 9.409 | 1.00 | 21.94 | N |
| ATOM | 220 | CA | TYR | A | 33 | 22.095 | 2.002 | 8.043 | 1.00 | 22.18 | C |
| ATOM | 221 | C | TYR | A | 33 | 21.762 | 0.511 | 8.013 | 1.00 | 22.46 | C |
| ATOM | 222 | O | TYR | A | 33 | 22.098 | -0.234 | 8.941 | 1.00 | 22.12 | O |
| ATOM | 223 | CB | TYR | A | 33 | 23.451 | 2.223 | 7.366 | 1.00 | 22.08 | C |
| ATOM | 224 | CG | TYR | A | 33 | 23.885 | 3.670 | 7.262 | 1.00 | 22.16 | C |
| ATOM | 225 | CD1 | TYR | A | 33 | 24.529 | 4.308 | 8.327 | 1.00 | 21.73 | C |
| ATOM | 226 | CE1 | TYR | A | 33 | 24.936 | 5.634 | 8.230 | 1.00 | 22.02 | C |
| ATOM | 227 | CZ | TYR | A | 33 | 24.703 | 6.336 | 7.054 | 1.00 | 22.45 | C |
| ATOM | 228 | OH | TYR | A | 33 | 25.102 | 7.650 | 6.948 | 1.00 | 22.61 | O |
| ATOM | 229 | CE2 | TYR | A | 33 | 24.071 | 5.722 | 5.983 | 1.00 | 22.07 | C |
| ATOM | 230 | CD2 | TYR | A | 33 | 23.669 | 4.397 | 6.091 | 1.00 | 21.88 | C |
| ATOM | 231 | N | LYS | A | 34 | 21.091 | 0.091 | 6.943 | 1.00 | 22.96 | N |
| ATOM | 232 | CA | LYS | A | 34 | 20.920 | -1.324 | 6.630 | 1.00 | 23.53 | C |
| ATOM | 233 | C | LYS | A | 34 | 22.116 | -1.756 | 5.801 | 1.00 | 23.91 | C |
| ATOM | 234 | O | LYS | A | 34 | 22.378 | -1.186 | 4.740 | 1.00 | 24.04 | O |
| ATOM | 235 | CB | LYS | A | 34 | 19.634 | -1.552 | 5.840 | 1.00 | 23.47 | C |

FIG. 4D

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|--------|------|-------|---|
| ATOM | 236 | CG | LYS | A | 34 | 18.408 | -1.735 | 6.698 | 1.00 | 23.52 | C |
| ATOM | 237 | CD | LYS | A | 34 | 17.241 | -2.250 | 5.885 | 1.00 | 24.01 | C |
| ATOM | 238 | CE | LYS | A | 34 | 16.228 | -1.155 | 5.595 | 1.00 | 24.30 | C |
| ATOM | 239 | NZ | LYS | A | 34 | 14.931 | -1.719 | 5.123 | 1.00 | 24.31 | N |
| ATOM | 240 | N | GLY | A | 35 | 22.849 | -2.752 | 6.284 | 1.00 | 24.57 | N |
| ATOM | 241 | CA | GLY | A | 35 | 24.090 | -3.141 | 5.639 | 1.00 | 25.53 | C |
| ATOM | 242 | C | GLY | A | 35 | 24.414 | -4.618 | 5.655 | 1.00 | 26.05 | C |
| ATOM | 243 | O | GLY | A | 35 | 23.731 | -5.412 | 6.299 | 1.00 | 25.91 | O |
| ATOM | 244 | N | LEU | A | 36 | 25.468 | -4.979 | 4.926 | 1.00 | 26.86 | N |
| ATOM | 245 | CA | LEU | A | 36 | 25.939 | -6.357 | 4.866 | 1.00 | 27.53 | C |
| ATOM | 246 | C | LEU | A | 36 | 27.246 | -6.519 | 5.623 | 1.00 | 27.91 | C |
| ATOM | 247 | O | LEU | A | 36 | 28.161 | -5.706 | 5.488 | 1.00 | 27.81 | O |
| ATOM | 248 | CB | LEU | A | 36 | 26.125 | -6.815 | 3.417 | 1.00 | 27.59 | C |
| ATOM | 249 | CG | LEU | A | 36 | 24.887 | -7.235 | 2.617 | 1.00 | 27.75 | C |
| ATOM | 250 | CD1 | LEU | A | 36 | 25.220 | -7.268 | 1.139 | 1.00 | 27.96 | C |
| ATOM | 251 | CD2 | LEU | A | 36 | 24.327 | -8.578 | 3.070 | 1.00 | 27.64 | C |
| ATOM | 252 | N | TRP | A | 37 | 27.316 | -7.573 | 6.426 | 1.00 | 28.55 | N |
| ATOM | 253 | CA | TRP | A | 37 | 28.537 | -7.946 | 7.120 | 1.00 | 29.32 | C |
| ATOM | 254 | C | TRP | A | 37 | 29.161 | -9.136 | 6.393 | 1.00 | 29.56 | C |
| ATOM | 255 | O | TRP | A | 37 | 28.544 | -10.198 | 6.271 | 1.00 | 29.63 | O |
| ATOM | 256 | CB | TRP | A | 37 | 28.235 | -8.282 | 8.588 | 1.00 | 29.55 | C |
| ATOM | 257 | CG | TRP | A | 37 | 29.439 | -8.624 | 9.439 | 1.00 | 30.21 | C |
| ATOM | 258 | CD1 | TRP | A | 37 | 30.760 | -8.455 | 9.117 | 1.00 | 30.54 | C |
| ATOM | 259 | NE1 | TRP | A | 37 | 31.560 | -8.884 | 10.150 | 1.00 | 30.79 | N |
| ATOM | 260 | CE2 | TRP | A | 37 | 30.767 | -9.337 | 11.171 | 1.00 | 30.90 | C |
| ATOM | 261 | CD2 | TRP | A | 37 | 29.423 | -9.187 | 10.758 | 1.00 | 30.80 | C |
| ATOM | 262 | CE3 | TRP | A | 37 | 28.404 | -9.586 | 11.639 | 1.00 | 30.90 | C |
| ATOM | 263 | CZ3 | TRP | A | 37 | 28.755 | -10.112 | 12.880 | 1.00 | 30.91 | C |
| ATOM | 264 | CH2 | TRP | A | 37 | 30.101 | -10.247 | 13.256 | 1.00 | 31.12 | C |
| ATOM | 265 | CZ2 | TRP | A | 37 | 31.119 | -9.867 | 12.418 | 1.00 | 31.16 | C |
| ATOM | 266 | N | ILE | A | 38 | 30.377 | -8.937 | 5.894 | 1.00 | 29.84 | N |
| ATOM | 267 | CA | ILE | A | 38 | 31.122 | -9.989 | 5.213 | 1.00 | 30.12 | C |
| ATOM | 268 | C | ILE | A | 38 | 32.495 | -10.182 | 5.866 | 1.00 | 30.29 | C |
| ATOM | 269 | O | ILE | A | 38 | 33.462 | -9.502 | 5.505 | 1.00 | 30.21 | O |
| ATOM | 270 | CB | ILE | A | 38 | 31.262 | -9.667 | 3.708 | 1.00 | 30.15 | C |
| ATOM | 271 | N | PRO | A | 39 | 32.572 | -11.092 | 6.840 | 1.00 | 30.44 | N |
| ATOM | 272 | CA | PRO | A | 39 | 33.837 | -11.396 | 7.520 | 1.00 | 30.58 | C |
| ATOM | 273 | C | PRO | A | 39 | 34.744 | -12.276 | 6.662 | 1.00 | 30.72 | C |
| ATOM | 274 | O | PRO | A | 39 | 35.314 | -11.787 | 5.684 | 1.00 | 30.85 | O |
| ATOM | 275 | CB | PRO | A | 39 | 33.391 | -12.163 | 8.774 | 1.00 | 30.57 | C |
| ATOM | 276 | CG | PRO | A | 39 | 31.891 | -12.069 | 8.798 | 1.00 | 30.59 | C |
| ATOM | 277 | CD | PRO | A | 39 | 31.459 | -11.893 | 7.379 | 1.00 | 30.54 | C |
| ATOM | 278 | N | LYS | A | 43 | 33.389 | -16.832 | 3.414 | 1.00 | 34.01 | N |
| ATOM | 279 | CA | LYS | A | 43 | 32.664 | -16.229 | 2.301 | 1.00 | 33.97 | C |
| ATOM | 280 | C | LYS | A | 43 | 31.153 | -16.250 | 2.550 | 1.00 | 33.90 | C |
| ATOM | 281 | O | LYS | A | 43 | 30.432 | -17.097 | 2.012 | 1.00 | 34.06 | O |
| ATOM | 282 | CB | LYS | A | 43 | 33.011 | -16.939 | 0.988 | 1.00 | 33.94 | C |
| ATOM | 283 | N | VAL | A | 44 | 30.688 | -15.314 | 3.376 | 1.00 | 33.72 | N |
| ATOM | 284 | CA | VAL | A | 44 | 29.269 | -15.191 | 3.715 | 1.00 | 33.43 | C |
| ATOM | 285 | C | VAL | A | 44 | 28.879 | -13.723 | 3.941 | 1.00 | 33.19 | C |
| ATOM | 286 | O | VAL | A | 44 | 29.570 | -12.988 | 4.653 | 1.00 | 33.45 | O |
| ATOM | 287 | CB | VAL | A | 44 | 28.886 | -16.089 | 4.938 | 1.00 | 33.47 | C |
| ATOM | 288 | CG1 | VAL | A | 44 | 29.561 | -15.613 | 6.227 | 1.00 | 33.41 | C |
| ATOM | 289 | CG2 | VAL | A | 44 | 27.373 | -16.183 | 5.108 | 1.00 | 33.62 | C |
| ATOM | 290 | N | LYS | A | 45 | 27.781 | -13.304 | 3.315 | 1.00 | 32.62 | N |
| ATOM | 291 | CA | LYS | A | 45 | 27.285 | -11.935 | 3.448 | 1.00 | 31.95 | C |
| ATOM | 292 | C | LYS | A | 45 | 25.982 | -11.900 | 4.248 | 1.00 | 31.55 | C |
| ATOM | 293 | O | LYS | A | 45 | 24.954 | -12.413 | 3.800 | 1.00 | 31.42 | O |
| ATOM | 294 | CB | LYS | A | 45 | 27.093 | -11.299 | 2.069 | 1.00 | 32.12 | C |
| ATOM | 295 | CG | LYS | A | 45 | 28.393 | -10.981 | 1.338 | 1.00 | 31.98 | C |

FIG. 4E

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|--------|------|-------|---|
| ATOM | 296 | N | ILE | A | 46 | 26.038 | -11.295 | 5.433 | 1.00 | 31.01 | N |
| ATOM | 297 | CA | ILE | A | 46 | 24.899 | -11.261 | 6.353 | 1.00 | 30.53 | C |
| ATOM | 298 | C | ILE | A | 46 | 24.293 | -9.856 | 6.462 | 1.00 | 30.18 | C |
| ATOM | 299 | O | ILE | A | 46 | 25.002 | -8.899 | 6.787 | 1.00 | 30.09 | O |
| ATOM | 300 | CB | ILE | A | 46 | 25.307 | -11.778 | 7.765 | 1.00 | 30.44 | C |
| ATOM | 301 | CG1 | ILE | A | 46 | 25.978 | -13.152 | 7.679 | 1.00 | 30.56 | C |
| ATOM | 302 | CD1 | ILE | A | 46 | 27.075 | -13.372 | 8.709 | 1.00 | 30.37 | C |
| ATOM | 303 | CG2 | ILE | A | 46 | 24.097 | -11.845 | 8.693 | 1.00 | 30.32 | C |
| ATOM | 304 | N | PRO | A | 47 | 22.988 | -9.734 | 6.194 | 1.00 | 29.71 | N |
| ATOM | 305 | CA | PRO | A | 47 | 22.262 | -8.483 | 6.448 | 1.00 | 29.17 | C |
| ATOM | 306 | C | PRO | A | 47 | 22.389 | -8.085 | 7.915 | 1.00 | 28.54 | C |
| ATOM | 307 | O | PRO | A | 47 | 22.234 | -8.925 | 8.808 | 1.00 | 28.40 | O |
| ATOM | 308 | CB | PRO | A | 47 | 20.812 | -8.840 | 6.108 | 1.00 | 29.22 | C |
| ATOM | 309 | CG | PRO | A | 47 | 20.923 | -9.976 | 5.157 | 1.00 | 29.60 | C |
| ATOM | 310 | CD | PRO | A | 47 | 22.110 | -10.771 | 5.620 | 1.00 | 29.70 | C |
| ATOM | 311 | N | VAL | A | 48 | 22.685 | -6.812 | 8.150 | 1.00 | 27.79 | N |
| ATOM | 312 | CA | VAL | A | 48 | 23.035 | -6.334 | 9.481 | 1.00 | 26.99 | C |
| ATOM | 313 | C | VAL | A | 48 | 22.648 | -4.863 | 9.666 | 1.00 | 26.58 | C |
| ATOM | 314 | O | VAL | A | 48 | 22.428 | -4.143 | 8.688 | 1.00 | 26.41 | O |
| ATOM | 315 | CB | VAL | A | 48 | 24.551 | -6.597 | 9.769 | 1.00 | 26.88 | C |
| ATOM | 316 | CG1 | VAL | A | 48 | 25.412 | -5.349 | 9.556 | 1.00 | 26.52 | C |
| ATOM | 317 | CG2 | VAL | A | 48 | 24.746 | -7.193 | 11.149 | 1.00 | 26.78 | C |
| ATOM | 318 | N | ALA | A | 49 | 22.538 | -4.436 | 10.921 | 1.00 | 26.08 | N |
| ATOM | 319 | CA | ALA | A | 49 | 22.311 | -3.031 | 11.243 | 1.00 | 25.76 | C |
| ATOM | 320 | C | ALA | A | 49 | 23.628 | -2.351 | 11.620 | 1.00 | 25.45 | C |
| ATOM | 321 | O | ALA | A | 49 | 24.440 | -2.917 | 12.352 | 1.00 | 25.30 | O |
| ATOM | 322 | CB | ALA | A | 49 | 21.289 | -2.896 | 12.365 | 1.00 | 25.64 | C |
| ATOM | 323 | N | ILE | A | 50 | 23.839 | -1.145 | 11.100 | 1.00 | 25.22 | N |
| ATOM | 324 | CA | ILE | A | 50 | 25.047 | -0.375 | 11.388 | 1.00 | 24.92 | C |
| ATOM | 325 | C | ILE | A | 50 | 24.669 | 1.022 | 11.858 | 1.00 | 24.98 | C |
| ATOM | 326 | O | ILE | A | 50 | 23.987 | 1.754 | 11.142 | 1.00 | 24.99 | O |
| ATOM | 327 | CB | ILE | A | 50 | 25.969 | -0.292 | 10.143 | 1.00 | 24.84 | C |
| ATOM | 328 | CG1 | ILE | A | 50 | 26.370 | -1.690 | 9.663 | 1.00 | 24.62 | C |
| ATOM | 329 | CD1 | ILE | A | 50 | 26.345 | -1.847 | 8.169 | 1.00 | 24.45 | C |
| ATOM | 330 | CG2 | ILE | A | 50 | 27.212 | 0.548 | 10.440 | 1.00 | 24.57 | C |
| ATOM | 331 | N | LYS | A | 51 | 25.104 | 1.384 | 13.064 | 1.00 | 24.96 | N |
| ATOM | 332 | CA | LYS | A | 51 | 24.872 | 2.727 | 13.585 | 1.00 | 24.88 | C |
| ATOM | 333 | C | LYS | A | 51 | 26.168 | 3.527 | 13.667 | 1.00 | 25.02 | C |
| ATOM | 334 | O | LYS | A | 51 | 27.059 | 3.209 | 14.459 | 1.00 | 24.91 | O |
| ATOM | 335 | CB | LYS | A | 51 | 24.177 | 2.683 | 14.948 | 1.00 | 24.81 | C |
| ATOM | 336 | CG | LYS | A | 51 | 23.684 | 4.048 | 15.428 | 1.00 | 24.46 | C |
| ATOM | 337 | CD | LYS | A | 51 | 23.423 | 4.058 | 16.918 | 1.00 | 23.98 | C |
| ATOM | 338 | CE | LYS | A | 51 | 22.136 | 4.793 | 17.240 | 1.00 | 24.44 | C |
| ATOM | 339 | NZ | LYS | A | 51 | 20.944 | 3.912 | 17.088 | 1.00 | 24.60 | N |
| ATOM | 340 | N | GLU | A | 52 | 26.265 | 4.563 | 12.840 | 1.00 | 25.22 | N |
| ATOM | 341 | CA | GLU | A | 52 | 27.416 | 5.457 | 12.870 | 1.00 | 25.49 | C |
| ATOM | 342 | C | GLU | A | 52 | 27.112 | 6.680 | 13.720 | 1.00 | 25.56 | C |
| ATOM | 343 | O | GLU | A | 52 | 26.217 | 7.459 | 13.397 | 1.00 | 25.56 | O |
| ATOM | 344 | CB | GLU | A | 52 | 27.836 | 5.869 | 11.458 | 1.00 | 25.46 | C |
| ATOM | 345 | CG | GLU | A | 52 | 29.131 | 6.665 | 11.419 | 1.00 | 25.64 | C |
| ATOM | 346 | CD | GLU | A | 52 | 29.686 | 6.820 | 10.021 | 1.00 | 26.06 | C |
| ATOM | 347 | OE1 | GLU | A | 52 | 28.934 | 7.251 | 9.119 | 1.00 | 26.33 | O |
| ATOM | 348 | OE2 | GLU | A | 52 | 30.881 | 6.514 | 9.826 | 1.00 | 26.57 | O |
| ATOM | 349 | N | LEU | A | 53 | 27.865 | 6.835 | 14.806 | 1.00 | 25.93 | N |
| ATOM | 350 | CA | LEU | A | 53 | 27.695 | 7.960 | 15.722 | 1.00 | 26.28 | C |
| ATOM | 351 | C | LEU | A | 53 | 28.093 | 9.273 | 15.054 | 1.00 | 26.67 | C |
| ATOM | 352 | O | LEU | A | 53 | 28.993 | 9.298 | 14.207 | 1.00 | 26.73 | O |
| ATOM | 353 | CB | LEU | A | 53 | 28.493 | 7.739 | 17.013 | 1.00 | 26.26 | C |
| ATOM | 354 | CG | LEU | A | 53 | 28.203 | 6.499 | 17.874 | 1.00 | 25.99 | C |
| ATOM | 355 | CD1 | LEU | A | 53 | 29.026 | 6.547 | 19.152 | 1.00 | 25.76 | C |

FIG. 4F

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 356 | CD2 | LEU | A | 53 | 26.717 | 6.334 | 18.201 | 1.00 | 25.22 | C |
| ATOM | 357 | N | ARG | A | 54 | 27.416 | 10.354 | 15.440 | 1.00 | 26.99 | N |
| ATOM | 358 | CA | ARG | A | 54 | 27.547 | 11.648 | 14.762 | 1.00 | 27.40 | C |
| ATOM | 359 | C | ARG | A | 54 | 28.922 | 12.298 | 14.910 | 1.00 | 27.37 | C |
| ATOM | 360 | O | ARG | A | 54 | 29.485 | 12.793 | 13.933 | 1.00 | 27.33 | O |
| ATOM | 361 | CB | ARG | A | 54 | 26.439 | 12.619 | 15.195 | 1.00 | 27.61 | C |
| ATOM | 362 | CG | ARG | A | 54 | 26.112 | 12.602 | 16.682 | 1.00 | 28.23 | C |
| ATOM | 363 | CD | ARG | A | 54 | 25.970 | 13.980 | 17.297 | 1.00 | 29.16 | C |
| ATOM | 364 | NE | ARG | A | 54 | 24.622 | 14.221 | 17.806 | 1.00 | 29.84 | N |
| ATOM | 365 | CZ | ARG | A | 54 | 24.212 | 13.915 | 19.034 | 1.00 | 30.13 | C |
| ATOM | 366 | NH1 | ARG | A | 54 | 25.040 | 13.343 | 19.902 | 1.00 | 29.81 | N |
| ATOM | 367 | NH2 | ARG | A | 54 | 22.965 | 14.183 | 19.398 | 1.00 | 30.10 | N |
| ATOM | 368 | N | GLU | A | 55 | 29.458 | 12.293 | 16.126 | 1.00 | 27.50 | N |
| ATOM | 369 | CA | GLU | A | 55 | 30.733 | 12.949 | 16.401 | 1.00 | 27.75 | C |
| ATOM | 370 | C | GLU | A | 55 | 31.941 | 12.082 | 16.047 | 1.00 | 27.52 | C |
| ATOM | 371 | O | GLU | A | 55 | 31.885 | 10.855 | 16.133 | 1.00 | 27.53 | O |
| ATOM | 372 | CB | GLU | A | 55 | 30.804 | 13.391 | 17.864 | 1.00 | 27.86 | C |
| ATOM | 373 | CG | GLU | A | 55 | 31.440 | 14.758 | 18.062 | 1.00 | 28.71 | C |
| ATOM | 374 | CD | GLU | A | 55 | 30.638 | 15.876 | 17.423 | 1.00 | 29.44 | C |
| ATOM | 375 | OE1 | GLU | A | 55 | 31.133 | 16.472 | 16.444 | 1.00 | 29.52 | O |
| ATOM | 376 | OE2 | GLU | A | 55 | 29.511 | 16.153 | 17.894 | 1.00 | 29.93 | O |
| ATOM | 377 | N | ALA | A | 56 | 33.025 | 12.736 | 15.639 | 1.00 | 27.39 | N |
| ATOM | 378 | CA | ALA | A | 56 | 34.281 | 12.056 | 15.341 | 1.00 | 27.18 | C |
| ATOM | 379 | C | ALA | A | 56 | 35.075 | 11.871 | 16.625 | 1.00 | 27.07 | C |
| ATOM | 380 | O | ALA | A | 56 | 35.031 | 12.723 | 17.516 | 1.00 | 27.11 | O |
| ATOM | 381 | CB | ALA | A | 56 | 35.083 | 12.844 | 14.327 | 1.00 | 27.15 | C |
| ATOM | 382 | N | THR | A | 57 | 35.801 | 10.760 | 16.714 | 1.00 | 26.90 | N |
| ATOM | 383 | CA | THR | A | 57 | 36.483 | 10.379 | 17.953 | 1.00 | 26.74 | C |
| ATOM | 384 | C | THR | A | 57 | 37.999 | 10.255 | 17.799 | 1.00 | 26.58 | C |
| ATOM | 385 | O | THR | A | 57 | 38.504 | 9.988 | 16.708 | 1.00 | 26.61 | O |
| ATOM | 386 | CB | THR | A | 57 | 35.915 | 9.050 | 18.487 | 1.00 | 26.65 | C |
| ATOM | 387 | OG1 | THR | A | 57 | 35.978 | 8.058 | 17.455 | 1.00 | 26.93 | O |
| ATOM | 388 | CG2 | THR | A | 57 | 34.423 | 9.166 | 18.783 | 1.00 | 26.44 | C |
| ATOM | 389 | N | SER | A | 58 | 38.710 | 10.449 | 18.908 | 1.00 | 26.43 | N |
| ATOM | 390 | CA | SER | A | 58 | 40.156 | 10.253 | 18.965 | 1.00 | 26.28 | C |
| ATOM | 391 | C | SER | A | 58 | 40.470 | 8.818 | 19.403 | 1.00 | 26.29 | C |
| ATOM | 392 | O | SER | A | 58 | 39.589 | 8.133 | 19.925 | 1.00 | 26.21 | O |
| ATOM | 393 | CB | SER | A | 58 | 40.794 | 11.269 | 19.923 | 1.00 | 26.26 | C |
| ATOM | 394 | OG | SER | A | 58 | 40.450 | 11.006 | 21.273 | 1.00 | 25.83 | O |
| ATOM | 395 | N | PRO | A | 59 | 41.702 | 8.353 | 19.175 | 1.00 | 26.34 | N |
| ATOM | 396 | CA | PRO | A | 59 | 42.135 | 7.035 | 19.660 | 1.00 | 26.51 | C |
| ATOM | 397 | C | PRO | A | 59 | 42.071 | 6.890 | 21.184 | 1.00 | 26.85 | C |
| ATOM | 398 | O | PRO | A | 59 | 41.934 | 5.768 | 21.667 | 1.00 | 26.99 | O |
| ATOM | 399 | CB | PRO | A | 59 | 43.585 | 6.949 | 19.184 | 1.00 | 26.33 | C |
| ATOM | 400 | CG | PRO | A | 59 | 43.639 | 7.861 | 18.024 | 1.00 | 26.20 | C |
| ATOM | 401 | CD | PRO | A | 59 | 42.770 | 9.019 | 18.405 | 1.00 | 26.26 | C |
| ATOM | 402 | N | LYS | A | 60 | 42.170 | 7.998 | 21.916 | 1.00 | 27.14 | N |
| ATOM | 403 | CA | LYS | A | 60 | 42.016 | 7.986 | 23.369 | 1.00 | 27.39 | C |
| ATOM | 404 | C | LYS | A | 60 | 40.575 | 7.673 | 23.763 | 1.00 | 27.44 | C |
| ATOM | 405 | O | LYS | A | 60 | 40.331 | 6.898 | 24.692 | 1.00 | 27.55 | O |
| ATOM | 406 | CB | LYS | A | 60 | 42.447 | 9.325 | 23.972 | 1.00 | 27.46 | C |
| ATOM | 407 | CG | LYS | A | 60 | 42.583 | 9.306 | 25.488 | 1.00 | 28.00 | C |
| ATOM | 408 | CD | LYS | A | 60 | 42.869 | 10.693 | 26.034 | 1.00 | 28.93 | C |
| ATOM | 409 | CE | LYS | A | 60 | 43.871 | 10.640 | 27.177 | 1.00 | 29.23 | C |
| ATOM | 410 | NZ | LYS | A | 60 | 44.059 | 11.981 | 27.803 | 1.00 | 29.95 | N |
| ATOM | 411 | N | ALA | A | 61 | 39.630 | 8.284 | 23.052 | 1.00 | 27.44 | N |
| ATOM | 412 | CA | ALA | A | 61 | 38.206 | 8.077 | 23.298 | 1.00 | 27.57 | C |
| ATOM | 413 | C | ALA | A | 61 | 37.722 | 6.740 | 22.734 | 1.00 | 27.64 | C |
| ATOM | 414 | O | ALA | A | 61 | 36.712 | 6.202 | 23.186 | 1.00 | 27.63 | O |
| ATOM | 415 | CB | ALA | A | 61 | 37.398 | 9.227 | 22.722 | 1.00 | 27.47 | C |

FIG. 4G

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 416 | N | ASN | A | 62 | 38.451 | 6.215 | 21.750 | 1.00 | 27.74 | N |
| ATOM | 417 | CA | ASN | A | 62 | 38.147 | 4.919 | 21.146 | 1.00 | 27.81 | C |
| ATOM | 418 | C | ASN | A | 62 | 38.422 | 3.737 | 22.079 | 1.00 | 28.04 | C |
| ATOM | 419 | O | ASN | A | 62 | 37.747 | 2.708 | 21.995 | 1.00 | 28.04 | O |
| ATOM | 420 | CB | ASN | A | 62 | 38.904 | 4.750 | 19.825 | 1.00 | 27.69 | C |
| ATOM | 421 | CG | ASN | A | 62 | 38.184 | 5.397 | 18.641 | 1.00 | 27.43 | C |
| ATOM | 422 | OD1 | ASN | A | 62 | 38.733 | 5.486 | 17.546 | 1.00 | 27.39 | O |
| ATOM | 423 | ND2 | ASN | A | 62 | 36.953 | 5.844 | 18.858 | 1.00 | 27.18 | N |
| ATOM | 424 | N | LYS | A | 63 | 39.409 | 3.891 | 22.962 | 1.00 | 28.17 | N |
| ATOM | 425 | CA | LYS | A | 63 | 39.689 | 2.900 | 24.003 | 1.00 | 28.31 | C |
| ATOM | 426 | C | LYS | A | 63 | 38.604 | 2.948 | 25.069 | 1.00 | 28.13 | C |
| ATOM | 427 | O | LYS | A | 63 | 38.251 | 1.921 | 25.652 | 1.00 | 28.20 | O |
| ATOM | 428 | CB | LYS | A | 63 | 41.059 | 3.133 | 24.657 | 1.00 | 28.53 | C |
| ATOM | 429 | CG | LYS | A | 63 | 42.145 | 3.632 | 23.720 | 1.00 | 29.21 | C |
| ATOM | 430 | CD | LYS | A | 63 | 43.536 | 3.291 | 24.232 | 1.00 | 30.19 | C |
| ATOM | 431 | CE | LYS | A | 63 | 44.615 | 3.990 | 23.415 | 1.00 | 30.62 | C |
| ATOM | 432 | NZ | LYS | A | 63 | 44.634 | 3.538 | 21.990 | 1.00 | 31.28 | N |
| ATOM | 433 | N | GLU | A | 64 | 38.094 | 4.153 | 25.319 | 1.00 | 27.93 | N |
| ATOM | 434 | CA | GLU | A | 64 | 37.020 | 4.381 | 26.280 | 1.00 | 27.83 | C |
| ATOM | 435 | C | GLU | A | 64 | 35.699 | 3.799 | 25.775 | 1.00 | 27.57 | C |
| ATOM | 436 | O | GLU | A | 64 | 34.914 | 3.256 | 26.555 | 1.00 | 27.65 | O |
| ATOM | 437 | CB | GLU | A | 64 | 36.866 | 5.880 | 26.555 | 1.00 | 28.05 | C |
| ATOM | 438 | CG | GLU | A | 64 | 37.613 | 6.378 | 27.784 | 1.00 | 28.76 | C |
| ATOM | 439 | CD | GLU | A | 64 | 38.500 | 7.575 | 27.489 | 1.00 | 29.57 | C |
| ATOM | 440 | OE1 | GLU | A | 64 | 37.961 | 8.662 | 27.184 | 1.00 | 29.83 | O |
| ATOM | 441 | OE2 | GLU | A | 64 | 39.740 | 7.429 | 27.563 | 1.00 | 30.06 | O |
| ATOM | 442 | N | ILE | A | 65 | 35.468 | 3.915 | 24.469 | 1.00 | 27.10 | N |
| ATOM | 443 | CA | ILE | A | 65 | 34.265 | 3.382 | 23.833 | 1.00 | 26.79 | C |
| ATOM | 444 | C | ILE | A | 65 | 34.319 | 1.850 | 23.722 | 1.00 | 26.71 | C |
| ATOM | 445 | O | ILE | A | 65 | 33.310 | 1.174 | 23.944 | 1.00 | 26.61 | O |
| ATOM | 446 | CB | ILE | A | 65 | 34.032 | 4.066 | 22.452 | 1.00 | 26.69 | C |
| ATOM | 447 | CG1 | ILE | A | 65 | 33.404 | 5.452 | 22.646 | 1.00 | 26.51 | C |
| ATOM | 448 | CD1 | ILE | A | 65 | 33.810 | 6.480 | 21.600 | 1.00 | 26.15 | C |
| ATOM | 449 | CG2 | ILE | A | 65 | 33.156 | 3.208 | 21.538 | 1.00 | 26.44 | C |
| ATOM | 450 | N | LEU | A | 66 | 35.498 | 1.316 | 23.398 | 1.00 | 26.55 | N |
| ATOM | 451 | CA | LEU | A | 66 | 35.705 | -0.130 | 23.275 | 1.00 | 26.54 | C |
| ATOM | 452 | C | LEU | A | 66 | 35.515 | -0.865 | 24.605 | 1.00 | 26.56 | C |
| ATOM | 453 | O | LEU | A | 66 | 34.974 | -1.971 | 24.630 | 1.00 | 26.50 | O |
| ATOM | 454 | CB | LEU | A | 66 | 37.088 | -0.437 | 22.684 | 1.00 | 26.51 | C |
| ATOM | 455 | CG | LEU | A | 66 | 37.414 | -1.887 | 22.299 | 1.00 | 26.33 | C |
| ATOM | 456 | CD1 | LEU | A | 66 | 36.859 | -2.252 | 20.931 | 1.00 | 26.29 | C |
| ATOM | 457 | CD2 | LEU | A | 66 | 38.914 | -2.117 | 22.338 | 1.00 | 26.51 | C |
| ATOM | 458 | N | ASP | A | 67 | 35.957 | -0.241 | 25.698 | 1.00 | 26.48 | N |
| ATOM | 459 | CA | ASP | A | 67 | 35.749 | -0.774 | 27.044 | 1.00 | 26.50 | C |
| ATOM | 460 | C | ASP | A | 67 | 34.261 | -0.928 | 27.351 | 1.00 | 26.28 | C |
| ATOM | 461 | O | ASP | A | 67 | 33.853 | -1.899 | 27.990 | 1.00 | 26.56 | O |
| ATOM | 462 | CB | ASP | A | 67 | 36.401 | 0.133 | 28.093 | 1.00 | 26.74 | C |
| ATOM | 463 | CG | ASP | A | 67 | 37.902 | -0.083 | 28.211 | 1.00 | 27.46 | C |
| ATOM | 464 | OD1 | ASP | A | 67 | 38.393 | -1.177 | 27.841 | 1.00 | 27.71 | O |
| ATOM | 465 | OD2 | ASP | A | 67 | 38.670 | 0.793 | 28.671 | 1.00 | 27.91 | O |
| ATOM | 466 | N | GLU | A | 68 | 33.464 | 0.034 | 26.891 | 1.00 | 25.78 | N |
| ATOM | 467 | CA | GLU | A | 68 | 32.012 | -0.014 | 27.029 | 1.00 | 25.30 | C |
| ATOM | 468 | C | GLU | A | 68 | 31.381 | -0.976 | 26.025 | 1.00 | 24.91 | C |
| ATOM | 469 | O | GLU | A | 68 | 30.321 | -1.545 | 26.290 | 1.00 | 25.04 | O |
| ATOM | 470 | CB | GLU | A | 68 | 31.412 | 1.385 | 26.860 | 1.00 | 25.52 | C |
| ATOM | 471 | N | ALA | A | 69 | 32.035 | -1.151 | 24.879 | 1.00 | 24.34 | N |
| ATOM | 472 | CA | ALA | A | 69 | 31.558 | -2.056 | 23.835 | 1.00 | 23.87 | C |
| ATOM | 473 | C | ALA | A | 69 | 31.687 | -3.522 | 24.243 | 1.00 | 23.69 | C |
| ATOM | 474 | O | ALA | A | 69 | 30.874 | -4.360 | 23.843 | 1.00 | 23.53 | O |
| ATOM | 475 | CB | ALA | A | 69 | 32.297 | -1.801 | 22.529 | 1.00 | 23.87 | C |

FIG. 4H

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|--------|------|-------|---|
| ATOM | 476 | N | TYR | A | 70 | 32.711 | -3.825 | 25.039 | 1.00 | 23.46 | N |
| ATOM | 477 | CA | TYR | A | 70 | 32.927 | -5.184 | 25.529 | 1.00 | 23.29 | C |
| ATOM | 478 | C | TYR | A | 70 | 31.781 | -5.661 | 26.422 | 1.00 | 22.94 | C |
| ATOM | 479 | O | TYR | A | 70 | 31.283 | -6.771 | 26.243 | 1.00 | 22.72 | O |
| ATOM | 480 | CB | TYR | A | 70 | 34.274 | -5.303 | 26.251 | 1.00 | 23.45 | C |
| ATOM | 481 | CG | TYR | A | 70 | 35.452 | -5.516 | 25.322 | 1.00 | 23.79 | C |
| ATOM | 482 | CD1 | TYR | A | 70 | 36.552 | -4.659 | 25.354 | 1.00 | 24.15 | C |
| ATOM | 483 | CE1 | TYR | A | 70 | 37.640 | -4.848 | 24.505 | 1.00 | 24.42 | C |
| ATOM | 484 | CZ | TYR | A | 70 | 37.633 | -5.904 | 23.609 | 1.00 | 24.64 | C |
| ATOM | 485 | OH | TYR | A | 70 | 38.705 | -6.089 | 22.768 | 1.00 | 25.17 | O |
| ATOM | 486 | CE2 | TYR | A | 70 | 36.554 | -6.774 | 23.556 | 1.00 | 24.46 | C |
| ATOM | 487 | CD2 | TYR | A | 70 | 35.471 | -6.577 | 24.413 | 1.00 | 24.17 | C |
| ATOM | 488 | N | VAL | A | 71 | 31.361 | -4.812 | 27.361 | 1.00 | 22.73 | N |
| ATOM | 489 | CA | VAL | A | 71 | 30.232 | -5.123 | 28.245 | 1.00 | 22.60 | C |
| ATOM | 490 | C | VAL | A | 71 | 28.891 | -5.095 | 27.498 | 1.00 | 22.24 | C |
| ATOM | 491 | O | VAL | A | 71 | 27.947 | -5.789 | 27.883 | 1.00 | 22.18 | O |
| ATOM | 492 | CB | VAL | A | 71 | 30.209 | -4.222 | 29.526 | 1.00 | 22.72 | C |
| ATOM | 493 | CG1 | VAL | A | 71 | 29.394 | -2.946 | 29.316 | 1.00 | 23.15 | C |
| ATOM | 494 | CG2 | VAL | A | 71 | 29.677 | -4.998 | 30.720 | 1.00 | 22.88 | C |
| ATOM | 495 | N | MET | A | 72 | 28.830 | -4.305 | 26.428 | 1.00 | 21.84 | N |
| ATOM | 496 | CA | MET | A | 72 | 27.656 | -4.231 | 25.562 | 1.00 | 21.50 | C |
| ATOM | 497 | C | MET | A | 72 | 27.478 | -5.515 | 24.743 | 1.00 | 21.21 | C |
| ATOM | 498 | O | MET | A | 72 | 26.351 | -5.948 | 24.488 | 1.00 | 21.23 | O |
| ATOM | 499 | CB | MET | A | 72 | 27.768 | -3.025 | 24.624 | 1.00 | 21.61 | C |
| ATOM | 500 | CG | MET | A | 72 | 26.904 | -1.837 | 25.019 | 1.00 | 21.94 | C |
| ATOM | 501 | SD | MET | A | 72 | 27.649 | -0.233 | 24.642 | 1.00 | 22.75 | S |
| ATOM | 502 | CE | MET | A | 72 | 27.395 | -0.140 | 22.876 | 1.00 | 22.15 | C |
| ATOM | 503 | N | ALA | A | 73 | 28.595 | -6.114 | 24.337 | 1.00 | 20.68 | N |
| ATOM | 504 | CA | ALA | A | 73 | 28.582 | -7.336 | 23.533 | 1.00 | 20.30 | C |
| ATOM | 505 | C | ALA | A | 73 | 28.360 | -8.600 | 24.367 | 1.00 | 20.05 | C |
| ATOM | 506 | O | ALA | A | 73 | 28.024 | -9.658 | 23.826 | 1.00 | 19.98 | O |
| ATOM | 507 | CB | ALA | A | 73 | 29.868 | -7.450 | 22.740 | 1.00 | 20.23 | C |
| ATOM | 508 | N | SER | A | 74 | 28.552 | -8.487 | 25.678 | 1.00 | 19.70 | N |
| ATOM | 509 | CA | SER | A | 74 | 28.418 | -9.625 | 26.582 | 1.00 | 19.65 | C |
| ATOM | 510 | C | SER | A | 74 | 27.036 | -9.683 | 27.227 | 1.00 | 19.63 | C |
| ATOM | 511 | O | SER | A | 74 | 26.816 | -10.444 | 28.171 | 1.00 | 19.59 | O |
| ATOM | 512 | CB | SER | A | 74 | 29.497 | -9.568 | 27.663 | 1.00 | 19.64 | C |
| ATOM | 513 | OG | SER | A | 74 | 29.360 | -8.394 | 28.444 | 1.00 | 19.34 | O |
| ATOM | 514 | N | VAL | A | 75 | 26.110 | -8.875 | 26.714 | 1.00 | 19.56 | N |
| ATOM | 515 | CA | VAL | A | 75 | 24.753 | -8.820 | 27.247 | 1.00 | 19.62 | C |
| ATOM | 516 | C | VAL | A | 75 | 23.961 | -10.040 | 26.785 | 1.00 | 19.63 | C |
| ATOM | 517 | O | VAL | A | 75 | 23.721 | -10.234 | 25.592 | 1.00 | 19.87 | O |
| ATOM | 518 | CB | VAL | A | 75 | 24.051 | -7.484 | 26.892 | 1.00 | 19.56 | C |
| ATOM | 519 | CG1 | VAL | A | 75 | 22.548 | -7.609 | 26.995 | 1.00 | 19.64 | C |
| ATOM | 520 | CG2 | VAL | A | 75 | 24.544 | -6.376 | 27.811 | 1.00 | 19.28 | C |
| ATOM | 521 | N | ASP | A | 76 | 23.574 | -10.863 | 27.751 | 1.00 | 19.68 | N |
| ATOM | 522 | CA | ASP | A | 76 | 22.984 | -12.165 | 27.473 | 1.00 | 19.85 | C |
| ATOM | 523 | C | ASP | A | 76 | 21.602 | -12.285 | 28.106 | 1.00 | 19.56 | C |
| ATOM | 524 | O | ASP | A | 76 | 21.469 | -12.729 | 29.249 | 1.00 | 19.88 | O |
| ATOM | 525 | CB | ASP | A | 76 | 23.915 | -13.272 | 27.976 | 1.00 | 20.10 | C |
| ATOM | 526 | CG | ASP | A | 76 | 23.440 | -14.658 | 27.594 | 1.00 | 21.13 | C |
| ATOM | 527 | OD1 | ASP | A | 76 | 23.099 | -14.875 | 26.409 | 1.00 | 22.00 | O |
| ATOM | 528 | OD2 | ASP | A | 76 | 23.381 | -15.597 | 28.417 | 1.00 | 22.09 | O |
| ATOM | 529 | N | ASN | A | 77 | 20.586 | -11.869 | 27.351 | 1.00 | 18.92 | N |
| ATOM | 530 | CA | ASN | A | 77 | 19.190 | -11.898 | 27.786 | 1.00 | 18.24 | C |
| ATOM | 531 | C | ASN | A | 77 | 18.263 | -11.902 | 26.568 | 1.00 | 17.79 | C |
| ATOM | 532 | O | ASN | A | 77 | 18.519 | -11.184 | 25.602 | 1.00 | 17.62 | O |
| ATOM | 533 | CB | ASN | A | 77 | 18.879 | -10.694 | 28.684 | 1.00 | 18.12 | C |
| ATOM | 534 | CG | ASN | A | 77 | 17.521 | -10.798 | 29.357 | 1.00 | 17.98 | C |
| ATOM | 535 | OD1 | ASN | A | 77 | 16.498 | -10.402 | 28.792 | 1.00 | 17.52 | O |

FIG. 4I

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|--------|------|-------|---|
| ATOM | 536 | ND2 | ASN | A | 77 | 17.504 | -11.336 | 30.570 | 1.00 | 17.96 | N |
| ATOM | 537 | N | PRO | A | 78 | 17.196 | -12.701 | 26.608 | 1.00 | 17.55 | N |
| ATOM | 538 | CA | PRO | A | 78 | 16.241 | -12.777 | 25.490 | 1.00 | 17.35 | C |
| ATOM | 539 | C | PRO | A | 78 | 15.580 | -11.444 | 25.115 | 1.00 | 17.03 | C |
| ATOM | 540 | O | PRO | A | 78 | 15.050 | -11.334 | 24.011 | 1.00 | 17.06 | O |
| ATOM | 541 | CB | PRO | A | 78 | 15.178 | -13.759 | 26.002 | 1.00 | 17.38 | C |
| ATOM | 542 | CG | PRO | A | 78 | 15.868 | -14.558 | 27.055 | 1.00 | 17.33 | C |
| ATOM | 543 | CD | PRO | A | 78 | 16.821 | -13.609 | 27.709 | 1.00 | 17.45 | C |
| ATOM | 544 | N | HIS | A | 79 | 15.615 | -10.456 | 26.007 | 1.00 | 16.78 | N |
| ATOM | 545 | CA | HIS | A | 79 | 14.908 | -9.193 | 25.781 | 1.00 | 16.48 | C |
| ATOM | 546 | C | HIS | A | 79 | 15.818 | -7.961 | 25.750 | 1.00 | 16.20 | C |
| ATOM | 547 | O | HIS | A | 79 | 15.361 | -6.833 | 25.926 | 1.00 | 16.03 | O |
| ATOM | 548 | CB | HIS | A | 79 | 13.769 | -9.036 | 26.794 | 1.00 | 16.50 | C |
| ATOM | 549 | CG | HIS | A | 79 | 12.910 | -10.256 | 26.913 | 1.00 | 16.54 | C |
| ATOM | 550 | ND1 | HIS | A | 79 | 12.004 | -10.625 | 25.941 | 1.00 | 16.70 | N |
| ATOM | 551 | CE1 | HIS | A | 79 | 11.411 | -11.749 | 26.301 | 1.00 | 17.03 | C |
| ATOM | 552 | NE2 | HIS | A | 79 | 11.902 | -12.125 | 27.468 | 1.00 | 16.85 | N |
| ATOM | 553 | CD2 | HIS | A | 79 | 12.845 | -11.211 | 27.869 | 1.00 | 16.65 | C |
| ATOM | 554 | N | VAL | A | 80 | 17.108 | -8.190 | 25.522 | 1.00 | 16.05 | N |
| ATOM | 555 | CA | VAL | A | 80 | 18.059 | -7.110 | 25.267 | 1.00 | 16.06 | C |
| ATOM | 556 | C | VAL | A | 80 | 18.901 | -7.460 | 24.038 | 1.00 | 16.03 | C |
| ATOM | 557 | O | VAL | A | 80 | 19.465 | -8.554 | 23.951 | 1.00 | 15.94 | O |
| ATOM | 558 | CB | VAL | A | 80 | 18.991 | -6.827 | 26.480 | 1.00 | 15.93 | C |
| ATOM | 559 | CG1 | VAL | A | 80 | 19.733 | -5.514 | 26.289 | 1.00 | 16.08 | C |
| ATOM | 560 | CG2 | VAL | A | 80 | 18.213 | -6.794 | 27.793 | 1.00 | 16.22 | C |
| ATOM | 561 | N | CYS | A | 81 | 18.966 | -6.537 | 23.084 | 1.00 | 16.00 | N |
| ATOM | 562 | CA | CYS | A | 81 | 19.822 | -6.701 | 21.915 | 1.00 | 15.98 | C |
| ATOM | 563 | C | CYS | A | 81 | 21.281 | -6.567 | 22.320 | 1.00 | 16.16 | C |
| ATOM | 564 | O | CYS | A | 81 | 21.651 | -5.645 | 23.056 | 1.00 | 16.19 | O |
| ATOM | 565 | CB | CYS | A | 81 | 19.493 | -5.657 | 20.852 | 1.00 | 15.86 | C |
| ATOM | 566 | SG | CYS | A | 81 | 17.783 | -5.682 | 20.280 | 1.00 | 16.45 | S |
| ATOM | 567 | N | ARG | A | 82 | 22.107 | -7.496 | 21.849 | 1.00 | 16.32 | N |
| ATOM | 568 | CA | ARG | A | 82 | 23.538 | -7.431 | 22.103 | 1.00 | 16.37 | C |
| ATOM | 569 | C | ARG | A | 82 | 24.271 | -6.785 | 20.930 | 1.00 | 16.42 | C |
| ATOM | 570 | O | ARG | A | 82 | 23.775 | -6.783 | 19.798 | 1.00 | 16.36 | O |
| ATOM | 571 | CB | ARG | A | 82 | 24.104 | -8.819 | 22.435 | 1.00 | 16.43 | C |
| ATOM | 572 | CG | ARG | A | 82 | 24.212 | -9.779 | 21.262 | 1.00 | 17.04 | C |
| ATOM | 573 | CD | ARG | A | 82 | 24.861 | -11.117 | 21.606 | 1.00 | 17.08 | C |
| ATOM | 574 | NE | ARG | A | 82 | 26.310 | -10.999 | 21.752 | 1.00 | 16.95 | N |
| ATOM | 575 | CZ | ARG | A | 82 | 27.195 | -11.441 | 20.867 | 1.00 | 16.88 | C |
| ATOM | 576 | NH1 | ARG | A | 82 | 28.490 | -11.283 | 21.096 | 1.00 | 16.92 | N |
| ATOM | 577 | NH2 | ARG | A | 82 | 26.797 | -12.040 | 19.752 | 1.00 | 16.92 | N |
| ATOM | 578 | N | LEU | A | 83 | 25.440 | -6.218 | 21.217 | 1.00 | 16.39 | N |
| ATOM | 579 | CA | LEU | A | 83 | 26.304 | -5.659 | 20.189 | 1.00 | 16.29 | C |
| ATOM | 580 | C | LEU | A | 83 | 27.126 | -6.778 | 19.559 | 1.00 | 16.57 | C |
| ATOM | 581 | O | LEU | A | 83 | 27.807 | -7.528 | 20.262 | 1.00 | 16.60 | O |
| ATOM | 582 | CB | LEU | A | 83 | 27.215 | -4.579 | 20.785 | 1.00 | 16.22 | C |
| ATOM | 583 | CG | LEU | A | 83 | 28.004 | -3.684 | 19.823 | 1.00 | 15.85 | C |
| ATOM | 584 | CD1 | LEU | A | 83 | 27.071 | -2.807 | 18.993 | 1.00 | 15.73 | C |
| ATOM | 585 | CD2 | LEU | A | 83 | 29.006 | -2.838 | 20.584 | 1.00 | 15.19 | C |
| ATOM | 586 | N | LEU | A | 84 | 27.047 | -6.896 | 18.236 | 1.00 | 16.76 | N |
| ATOM | 587 | CA | LEU | A | 84 | 27.745 | -7.958 | 17.517 | 1.00 | 17.01 | C |
| ATOM | 588 | C | LEU | A | 84 | 29.176 | -7.563 | 17.165 | 1.00 | 17.23 | C |
| ATOM | 589 | O | LEU | A | 84 | 30.108 | -8.351 | 17.349 | 1.00 | 17.18 | O |
| ATOM | 590 | CB | LEU | A | 84 | 26.978 | -8.370 | 16.252 | 1.00 | 17.03 | C |
| ATOM | 591 | CG | LEU | A | 84 | 25.513 | -8.812 | 16.363 | 1.00 | 17.02 | C |
| ATOM | 592 | CD1 | LEU | A | 84 | 24.934 | -9.026 | 14.978 | 1.00 | 16.99 | C |
| ATOM | 593 | CD2 | LEU | A | 84 | 25.355 | -10.076 | 17.200 | 1.00 | 17.18 | C |
| ATOM | 594 | N | GLY | A | 85 | 29.343 | -6.342 | 16.664 | 1.00 | 17.48 | N |
| ATOM | 595 | CA | GLY | A | 85 | 30.644 | -5.859 | 16.239 | 1.00 | 17.82 | C |

FIG. 4J

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 596 | C | GLY | A | 85 | 30.819 | -4.359 | 16.362 | 1.00 | 18.07 | C |
| ATOM | 597 | O | GLY | A | 85 | 29.864 | -3.624 | 16.636 | 1.00 | 18.08 | O |
| ATOM | 598 | N | ILE | A | 86 | 32.054 | -3.909 | 16.155 | 1.00 | 18.32 | N |
| ATOM | 599 | CA | ILE | A | 86 | 32.396 | -2.487 | 16.211 | 1.00 | 18.48 | C |
| ATOM | 600 | C | ILE | A | 86 | 33.548 | -2.160 | 15.257 | 1.00 | 18.45 | C |
| ATOM | 601 | O | ILE | A | 86 | 34.468 | -2.962 | 15.088 | 1.00 | 18.58 | O |
| ATOM | 602 | CB | ILE | A | 86 | 32.715 | -2.051 | 17.680 | 1.00 | 18.40 | C |
| ATOM | 603 | CG1 | ILE | A | 86 | 32.659 | -0.527 | 17.827 | 1.00 | 18.47 | C |
| ATOM | 604 | CD1 | ILE | A | 86 | 32.054 | -0.048 | 19.136 | 1.00 | 18.61 | C |
| ATOM | 605 | CG2 | ILE | A | 86 | 34.048 | -2.634 | 18.172 | 1.00 | 18.36 | C |
| ATOM | 606 | N | CYS | A | 87 | 33.474 | -0.991 | 14.625 | 1.00 | 18.51 | N |
| ATOM | 607 | CA | CYS | A | 87 | 34.562 | -0.470 | 13.803 | 1.00 | 18.57 | C |
| ATOM | 608 | C | CYS | A | 87 | 35.006 | 0.883 | 14.344 | 1.00 | 18.66 | C |
| ATOM | 609 | O | CYS | A | 87 | 34.233 | 1.843 | 14.338 | 1.00 | 18.66 | O |
| ATOM | 610 | CB | CYS | A | 87 | 34.120 | -0.335 | 12.347 | 1.00 | 18.69 | C |
| ATOM | 611 | SG | CYS | A | 87 | 35.452 | 0.059 | 11.185 | 1.00 | 19.10 | S |
| ATOM | 612 | N | LEU | A | 88 | 36.248 | 0.952 | 14.819 | 1.00 | 18.94 | N |
| ATOM | 613 | CA | LEU | A | 88 | 36.782 | 2.182 | 15.407 | 1.00 | 19.23 | C |
| ATOM | 614 | C | LEU | A | 88 | 37.864 | 2.823 | 14.541 | 1.00 | 19.32 | C |
| ATOM | 615 | O | LEU | A | 88 | 39.016 | 2.384 | 14.526 | 1.00 | 19.42 | O |
| ATOM | 616 | CB | LEU | A | 88 | 37.297 | 1.942 | 16.833 | 1.00 | 19.16 | C |
| ATOM | 617 | CG | LEU | A | 88 | 36.265 | 1.583 | 17.911 | 1.00 | 19.62 | C |
| ATOM | 618 | CD1 | LEU | A | 88 | 36.939 | 0.968 | 19.127 | 1.00 | 19.50 | C |
| ATOM | 619 | CD2 | LEU | A | 88 | 35.440 | 2.788 | 18.325 | 1.00 | 19.54 | C |
| ATOM | 620 | N | THR | A | 89 | 37.464 | 3.858 | 13.811 | 1.00 | 19.57 | N |
| ATOM | 621 | CA | THR | A | 89 | 38.380 | 4.679 | 13.028 | 1.00 | 19.85 | C |
| ATOM | 622 | C | THR | A | 89 | 38.328 | 6.101 | 13.593 | 1.00 | 19.94 | C |
| ATOM | 623 | O | THR | A | 89 | 38.535 | 6.296 | 14.793 | 1.00 | 19.99 | O |
| ATOM | 624 | CB | THR | A | 89 | 38.001 | 4.646 | 11.528 | 1.00 | 19.89 | C |
| ATOM | 625 | OG1 | THR | A | 89 | 36.581 | 4.785 | 11.381 | 1.00 | 20.27 | O |
| ATOM | 626 | CG2 | THR | A | 89 | 38.284 | 3.278 | 10.929 | 1.00 | 19.88 | C |
| ATOM | 627 | N | SER | A | 90 | 38.049 | 7.088 | 12.743 | 1.00 | 19.99 | N |
| ATOM | 628 | CA | SER | A | 90 | 37.726 | 8.432 | 13.219 | 1.00 | 20.17 | C |
| ATOM | 629 | C | SER | A | 90 | 36.265 | 8.464 | 13.666 | 1.00 | 20.14 | C |
| ATOM | 630 | O | SER | A | 90 | 35.877 | 9.292 | 14.491 | 1.00 | 20.44 | O |
| ATOM | 631 | CB | SER | A | 90 | 37.977 | 9.482 | 12.139 | 1.00 | 20.18 | C |
| ATOM | 632 | OG | SER | A | 90 | 37.379 | 9.104 | 10.911 | 1.00 | 20.96 | O |
| ATOM | 633 | N | THR | A | 91 | 35.468 | 7.549 | 13.116 | 1.00 | 19.87 | N |
| ATOM | 634 | CA | THR | A | 91 | 34.072 | 7.382 | 13.510 | 1.00 | 19.58 | C |
| ATOM | 635 | C | THR | A | 91 | 33.856 | 6.044 | 14.216 | 1.00 | 19.51 | C |
| ATOM | 636 | O | THR | A | 91 | 34.613 | 5.085 | 14.010 | 1.00 | 19.54 | O |
| ATOM | 637 | CB | THR | A | 91 | 33.130 | 7.486 | 12.288 | 1.00 | 19.65 | C |
| ATOM | 638 | OG1 | THR | A | 91 | 33.410 | 6.422 | 11.368 | 1.00 | 19.55 | O |
| ATOM | 639 | CG2 | THR | A | 91 | 33.412 | 8.750 | 11.481 | 1.00 | 19.51 | C |
| ATOM | 640 | N | VAL | A | 92 | 32.821 | 5.999 | 15.051 | 1.00 | 19.08 | N |
| ATOM | 641 | CA | VAL | A | 92 | 32.411 | 4.786 | 15.748 | 1.00 | 18.72 | C |
| ATOM | 642 | C | VAL | A | 92 | 31.215 | 4.192 | 15.015 | 1.00 | 18.52 | C |
| ATOM | 643 | O | VAL | A | 92 | 30.201 | 4.872 | 14.811 | 1.00 | 18.23 | O |
| ATOM | 644 | CB | VAL | A | 92 | 32.036 | 5.079 | 17.224 | 1.00 | 18.93 | C |
| ATOM | 645 | CG1 | VAL | A | 92 | 31.485 | 3.833 | 17.917 | 1.00 | 18.55 | C |
| ATOM | 646 | CG2 | VAL | A | 92 | 33.236 | 5.635 | 17.983 | 1.00 | 19.17 | C |
| ATOM | 647 | N | GLN | A | 93 | 31.340 | 2.929 | 14.612 | 1.00 | 18.15 | N |
| ATOM | 648 | CA | GLN | A | 93 | 30.278 | 2.259 | 13.866 | 1.00 | 18.10 | C |
| ATOM | 649 | C | GLN | A | 93 | 29.852 | 0.965 | 14.555 | 1.00 | 17.96 | C |
| ATOM | 650 | O | GLN | A | 93 | 30.594 | -0.019 | 14.575 | 1.00 | 18.09 | O |
| ATOM | 651 | CB | GLN | A | 93 | 30.698 | 2.016 | 12.410 | 1.00 | 18.03 | C |
| ATOM | 652 | CG | GLN | A | 93 | 30.900 | 3.296 | 11.608 | 1.00 | 17.82 | C |
| ATOM | 653 | CD | GLN | A | 93 | 31.124 | 3.043 | 10.133 | 1.00 | 18.23 | C |
| ATOM | 654 | OE1 | GLN | A | 93 | 30.168 | 2.847 | 9.383 | 1.00 | 18.82 | O |
| ATOM | 655 | NE2 | GLN | A | 93 | 32.383 | 3.056 | 9.709 | 1.00 | 17.84 | N |

FIG. 4K

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 656 | N | LEU | A | 94 | 28.651 | 0.988 | 15.126 | 1.00 | 17.85 | N |
| ATOM | 657 | CA | LEU | A | 94 | 28.125 | -0.128 | 15.906 | 1.00 | 17.83 | C |
| ATOM | 658 | C | LEU | A | 94 | 27.372 | -1.111 | 15.017 | 1.00 | 17.85 | C |
| ATOM | 659 | O | LEU | A | 94 | 26.526 | -0.711 | 14.214 | 1.00 | 17.77 | O |
| ATOM | 660 | CB | LEU | A | 94 | 27.208 | 0.382 | 17.023 | 1.00 | 17.79 | C |
| ATOM | 661 | CG | LEU | A | 94 | 27.785 | 1.411 | 18.001 | 1.00 | 18.19 | C |
| ATOM | 662 | CD1 | LEU | A | 94 | 26.729 | 2.434 | 18.385 | 1.00 | 18.54 | C |
| ATOM | 663 | CD2 | LEU | A | 94 | 28.355 | 0.743 | 19.242 | 1.00 | 18.09 | C |
| ATOM | 664 | N | ILE | A | 95 | 27.683 | -2.396 | 15.167 | 1.00 | 17.79 | N |
| ATOM | 665 | CA | ILE | A | 95 | 27.047 | -3.438 | 14.364 | 1.00 | 17.61 | C |
| ATOM | 666 | C | ILE | A | 95 | 26.143 | -4.321 | 15.223 | 1.00 | 17.27 | C |
| ATOM | 667 | O | ILE | A | 95 | 26.604 | -4.997 | 16.142 | 1.00 | 17.09 | O |
| ATOM | 668 | CB | ILE | A | 95 | 28.112 | -4.263 | 13.577 | 1.00 | 17.84 | C |
| ATOM | 669 | CG1 | ILE | A | 95 | 28.764 | -3.398 | 12.495 | 1.00 | 17.99 | C |
| ATOM | 670 | CD1 | ILE | A | 95 | 30.161 | -2.931 | 12.843 | 1.00 | 19.08 | C |
| ATOM | 671 | CG2 | ILE | A | 95 | 27.493 | -5.498 | 12.926 | 1.00 | 17.50 | C |
| ATOM | 672 | N | THR | A | 96 | 24.849 | -4.285 | 14.915 | 1.00 | 17.10 | N |
| ATOM | 673 | CA | THR | A | 96 | 23.843 | -5.096 | 15.598 | 1.00 | 17.04 | C |
| ATOM | 674 | C | THR | A | 96 | 23.044 | -5.906 | 14.588 | 1.00 | 17.16 | C |
| ATOM | 675 | O | THR | A | 96 | 23.148 | -5.685 | 13.378 | 1.00 | 17.06 | O |
| ATOM | 676 | CB | THR | A | 96 | 22.871 | -4.216 | 16.417 | 1.00 | 16.89 | C |
| ATOM | 677 | OG1 | THR | A | 96 | 22.467 | -3.090 | 15.630 | 1.00 | 17.74 | O |
| ATOM | 678 | CG2 | THR | A | 96 | 23.563 | -3.594 | 17.627 | 1.00 | 16.46 | C |
| ATOM | 679 | N | GLN | A | 97 | 22.245 | -6.841 | 15.098 | 1.00 | 17.15 | N |
| ATOM | 680 | CA | GLN | A | 97 | 21.337 | -7.632 | 14.282 | 1.00 | 17.15 | C |
| ATOM | 681 | C | GLN | A | 97 | 20.247 | -6.754 | 13.668 | 1.00 | 17.13 | C |
| ATOM | 682 | O | GLN | A | 97 | 19.576 | -5.989 | 14.374 | 1.00 | 16.94 | O |
| ATOM | 683 | CB | GLN | A | 97 | 20.702 | -8.732 | 15.133 | 1.00 | 17.29 | C |
| ATOM | 684 | CG | GLN | A | 97 | 19.940 | -9.788 | 14.351 | 1.00 | 18.00 | C |
| ATOM | 685 | CD | GLN | A | 97 | 19.295 | -10.832 | 15.246 | 1.00 | 19.09 | C |
| ATOM | 686 | OE1 | GLN | A | 97 | 19.522 | -10.849 | 16.458 | 1.00 | 20.02 | O |
| ATOM | 687 | NE2 | GLN | A | 97 | 18.484 | -11.703 | 14.653 | 1.00 | 19.24 | N |
| ATOM | 688 | N | LEU | A | 98 | 20.090 | -6.863 | 12.351 | 1.00 | 17.04 | N |
| ATOM | 689 | CA | LEU | A | 98 | 19.015 | -6.184 | 11.636 | 1.00 | 17.05 | C |
| ATOM | 690 | C | LEU | A | 98 | 17.678 | -6.803 | 12.019 | 1.00 | 17.14 | C |
| ATOM | 691 | O | LEU | A | 98 | 17.535 | -8.027 | 12.052 | 1.00 | 17.33 | O |
| ATOM | 692 | CB | LEU | A | 98 | 19.233 | -6.259 | 10.119 | 1.00 | 16.85 | C |
| ATOM | 693 | CG | LEU | A | 98 | 18.191 | -5.635 | 9.179 | 1.00 | 16.81 | C |
| ATOM | 694 | CD1 | LEU | A | 98 | 17.866 | -4.182 | 9.546 | 1.00 | 16.35 | C |
| ATOM | 695 | CD2 | LEU | A | 98 | 18.647 | -5.745 | 7.721 | 1.00 | 16.48 | C |
| ATOM | 696 | N | MET | A | 99 | 16.708 | -5.943 | 12.311 | 1.00 | 17.24 | N |
| ATOM | 697 | CA | MET | A | 99 | 15.401 | -6.375 | 12.784 | 1.00 | 17.22 | C |
| ATOM | 698 | C | MET | A | 99 | 14.316 | -5.915 | 11.819 | 1.00 | 17.29 | C |
| ATOM | 699 | O | MET | A | 99 | 13.894 | -4.757 | 11.862 | 1.00 | 17.57 | O |
| ATOM | 700 | CB | MET | A | 99 | 15.140 | -5.840 | 14.195 | 1.00 | 17.43 | C |
| ATOM | 701 | CG | MET | A | 99 | 16.186 | -6.255 | 15.218 | 1.00 | 17.31 | C |
| ATOM | 702 | SD | MET | A | 99 | 15.708 | -7.745 | 16.087 | 1.00 | 17.72 | S |
| ATOM | 703 | CE | MET | A | 99 | 16.339 | -9.005 | 15.021 | 1.00 | 18.23 | C |
| ATOM | 704 | N | PRO | A | 100 | 13.871 | -6.827 | 10.953 | 1.00 | 17.17 | N |
| ATOM | 705 | CA | PRO | A | 100 | 12.919 | -6.506 | 9.881 | 1.00 | 16.97 | C |
| ATOM | 706 | C | PRO | A | 100 | 11.707 | -5.698 | 10.338 | 1.00 | 16.82 | C |
| ATOM | 707 | O | PRO | A | 100 | 11.305 | -4.766 | 9.642 | 1.00 | 16.79 | O |
| ATOM | 708 | CB | PRO | A | 100 | 12.467 | -7.889 | 9.392 | 1.00 | 17.04 | C |
| ATOM | 709 | CG | PRO | A | 100 | 13.611 | -8.790 | 9.692 | 1.00 | 16.92 | C |
| ATOM | 710 | CD | PRO | A | 100 | 14.256 | -8.252 | 10.939 | 1.00 | 17.04 | C |
| ATOM | 711 | N | PHE | A | 101 | 11.147 | -6.042 | 11.494 | 1.00 | 16.80 | N |
| ATOM | 712 | CA | PHE | A | 101 | 9.869 | -5.473 | 11.928 | 1.00 | 16.70 | C |
| ATOM | 713 | C | PHE | A | 101 | 9.994 | -4.135 | 12.660 | 1.00 | 16.47 | C |
| ATOM | 714 | O | PHE | A | 101 | 8.985 | -3.498 | 12.971 | 1.00 | 16.61 | O |
| ATOM | 715 | CB | PHE | A | 101 | 9.089 | -6.496 | 12.764 | 1.00 | 16.80 | C |

FIG. 4L

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 716 | CG | PHE | A | 101 | 9.063 | -7.875 | 12.160 | 1.00 | 17.13 | C |
| ATOM | 717 | CD1 | PHE | A | 101 | 8.617 | -8.073 | 10.852 | 1.00 | 17.47 | C |
| ATOM | 718 | CE1 | PHE | A | 101 | 8.600 | -9.344 | 10.286 | 1.00 | 17.80 | C |
| ATOM | 719 | CZ | PHE | A | 101 | 9.032 | -10.437 | 11.031 | 1.00 | 17.99 | C |
| ATOM | 720 | CE2 | PHE | A | 101 | 9.482 | -10.252 | 12.340 | 1.00 | 17.77 | C |
| ATOM | 721 | CD2 | PHE | A | 101 | 9.495 | -8.975 | 12.894 | 1.00 | 17.36 | C |
| ATOM | 722 | N | GLY | A | 102 | 11.231 | -3.717 | 12.926 | 1.00 | 16.07 | N |
| ATOM | 723 | CA | GLY | A | 102 | 11.499 | -2.428 | 13.539 | 1.00 | 15.74 | C |
| ATOM | 724 | C | GLY | A | 102 | 11.060 | -2.335 | 14.988 | 1.00 | 15.51 | C |
| ATOM | 725 | O | GLY | A | 102 | 10.991 | -3.348 | 15.688 | 1.00 | 15.56 | O |
| ATOM | 726 | N | CYS | A | 103 | 10.748 | -1.115 | 15.424 | 1.00 | 15.09 | N |
| ATOM | 727 | CA | CYS | A | 103 | 10.420 | -0.837 | 16.820 | 1.00 | 14.69 | C |
| ATOM | 728 | C | CYS | A | 103 | 8.946 | -1.051 | 17.182 | 1.00 | 14.97 | C |
| ATOM | 729 | O | CYS | A | 103 | 8.082 | -1.145 | 16.308 | 1.00 | 15.08 | O |
| ATOM | 730 | CB | CYS | A | 103 | 10.858 | 0.581 | 17.193 | 1.00 | 14.64 | C |
| ATOM | 731 | SG | CYS | A | 103 | 9.883 | 1.905 | 16.452 | 1.00 | 12.98 | S |
| ATOM | 732 | N | LEU | A | 104 | 8.681 | -1.127 | 18.485 | 1.00 | 15.04 | N |
| ATOM | 733 | CA | LEU | A | 104 | 7.341 | -1.367 | 19.016 | 1.00 | 15.24 | C |
| ATOM | 734 | C | LEU | A | 104 | 6.437 | -0.141 | 18.910 | 1.00 | 15.61 | C |
| ATOM | 735 | O | LEU | A | 104 | 5.214 | -0.280 | 18.815 | 1.00 | 15.55 | O |
| ATOM | 736 | CB | LEU | A | 104 | 7.430 | -1.847 | 20.473 | 1.00 | 15.21 | C |
| ATOM | 737 | CG | LEU | A | 104 | 6.260 | -2.575 | 21.147 | 1.00 | 14.92 | C |
| ATOM | 738 | CD1 | LEU | A | 104 | 5.811 | -3.816 | 20.378 | 1.00 | 14.92 | C |
| ATOM | 739 | CD2 | LEU | A | 104 | 6.644 | -2.949 | 22.566 | 1.00 | 14.68 | C |
| ATOM | 740 | N | LEU | A | 105 | 7.039 | 1.051 | 18.931 | 1.00 | 15.86 | N |
| ATOM | 741 | CA | LEU | A | 105 | 6.289 | 2.300 | 18.796 | 1.00 | 16.29 | C |
| ATOM | 742 | C | LEU | A | 105 | 5.565 | 2.395 | 17.449 | 1.00 | 16.67 | C |
| ATOM | 743 | O | LEU | A | 105 | 4.396 | 2.785 | 17.394 | 1.00 | 16.80 | O |
| ATOM | 744 | CB | LEU | A | 105 | 7.191 | 3.525 | 19.017 | 1.00 | 16.11 | C |
| ATOM | 745 | CG | LEU | A | 105 | 6.552 | 4.907 | 18.805 | 1.00 | 16.10 | C |
| ATOM | 746 | CD1 | LEU | A | 105 | 5.445 | 5.170 | 19.817 | 1.00 | 15.96 | C |
| ATOM | 747 | CD2 | LEU | A | 105 | 7.591 | 6.020 | 18.841 | 1.00 | 15.85 | C |
| ATOM | 748 | N | ASP | A | 106 | 6.260 | 2.039 | 16.372 | 1.00 | 17.10 | N |
| ATOM | 749 | CA | ASP | A | 106 | 5.658 | 2.012 | 15.042 | 1.00 | 17.60 | C |
| ATOM | 750 | C | ASP | A | 106 | 4.586 | 0.933 | 14.951 | 1.00 | 17.69 | C |
| ATOM | 751 | O | ASP | A | 106 | 3.544 | 1.135 | 14.325 | 1.00 | 17.84 | O |
| ATOM | 752 | CB | ASP | A | 106 | 6.722 | 1.770 | 13.972 | 1.00 | 17.85 | C |
| ATOM | 753 | CG | ASP | A | 106 | 7.574 | 2.995 | 13.703 | 1.00 | 18.72 | C |
| ATOM | 754 | OD1 | ASP | A | 106 | 8.698 | 2.820 | 13.184 | 1.00 | 19.86 | O |
| ATOM | 755 | OD2 | ASP | A | 106 | 7.212 | 4.164 | 13.968 | 1.00 | 19.60 | O |
| ATOM | 756 | N | TYR | A | 107 | 4.852 | -0.205 | 15.589 | 1.00 | 17.77 | N |
| ATOM | 757 | CA | TYR | A | 107 | 3.956 | -1.355 | 15.567 | 1.00 | 18.06 | C |
| ATOM | 758 | C | TYR | A | 107 | 2.599 | -1.049 | 16.199 | 1.00 | 18.45 | C |
| ATOM | 759 | O | TYR | A | 107 | 1.559 | -1.386 | 15.626 | 1.00 | 18.63 | O |
| ATOM | 760 | CB | TYR | A | 107 | 4.612 | -2.561 | 16.255 | 1.00 | 17.90 | C |
| ATOM | 761 | CG | TYR | A | 107 | 3.800 | -3.834 | 16.181 | 1.00 | 17.51 | C |
| ATOM | 762 | CD1 | TYR | A | 107 | 3.975 | -4.735 | 15.133 | 1.00 | 17.26 | C |
| ATOM | 763 | CE1 | TYR | A | 107 | 3.229 | -5.907 | 15.061 | 1.00 | 17.00 | C |
| ATOM | 764 | CZ | TYR | A | 107 | 2.296 | -6.185 | 16.045 | 1.00 | 16.88 | C |
| ATOM | 765 | OH | TYR | A | 107 | 1.557 | -7.340 | 15.981 | 1.00 | 16.84 | O |
| ATOM | 766 | CE2 | TYR | A | 107 | 2.103 | -5.307 | 17.094 | 1.00 | 17.36 | C |
| ATOM | 767 | CD2 | TYR | A | 107 | 2.855 | -4.138 | 17.160 | 1.00 | 17.47 | C |
| ATOM | 768 | N | VAL | A | 108 | 2.615 | -0.416 | 17.372 | 1.00 | 18.85 | N |
| ATOM | 769 | CA | VAL | A | 108 | 1.380 | -0.072 | 18.078 | 1.00 | 19.41 | C |
| ATOM | 770 | C | VAL | A | 108 | 0.592 | 1.032 | 17.360 | 1.00 | 19.97 | C |
| ATOM | 771 | O | VAL | A | 108 | -0.640 | 1.055 | 17.409 | 1.00 | 19.85 | O |
| ATOM | 772 | CB | VAL | A | 108 | 1.615 | 0.288 | 19.580 | 1.00 | 19.29 | C |
| ATOM | 773 | CG1 | VAL | A | 108 | 2.162 | -0.910 | 20.343 | 1.00 | 18.99 | C |
| ATOM | 774 | CG2 | VAL | A | 108 | 2.532 | 1.496 | 19.741 | 1.00 | 19.23 | C |
| ATOM | 775 | N | ARG | A | 109 | 1.312 | 1.927 | 16.685 | 1.00 | 20.66 | N |

FIG. 4M

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 776 | CA | ARG | A | 109 | 0.694 | 2.985 | 15.891 | 1.00 | 21.58 | C |
| ATOM | 777 | C | ARG | A | 109 | -0.029 | 2.421 | 14.669 | 1.00 | 22.30 | C |
| ATOM | 778 | O | ARG | A | 109 | -1.102 | 2.904 | 14.306 | 1.00 | 22.64 | O |
| ATOM | 779 | CB | ARG | A | 109 | 1.734 | 4.018 | 15.459 | 1.00 | 21.32 | C |
| ATOM | 780 | CG | ARG | A | 109 | 2.024 | 5.069 | 16.511 | 1.00 | 20.85 | C |
| ATOM | 781 | CD | ARG | A | 109 | 3.315 | 5.823 | 16.284 | 1.00 | 20.35 | C |
| ATOM | 782 | NE | ARG | A | 109 | 3.536 | 6.834 | 17.313 | 1.00 | 19.97 | N |
| ATOM | 783 | CZ | ARG | A | 109 | 4.261 | 7.935 | 17.147 | 1.00 | 19.50 | C |
| ATOM | 784 | NH1 | ARG | A | 109 | 4.848 | 8.186 | 15.983 | 1.00 | 18.73 | N |
| ATOM | 785 | NH2 | ARG | A | 109 | 4.397 | 8.791 | 18.150 | 1.00 | 19.22 | N |
| ATOM | 786 | N | GLU | A | 110 | 0.560 | 1.399 | 14.047 | 1.00 | 23.05 | N |
| ATOM | 787 | CA | GLU | A | 110 | -0.053 | 0.732 | 12.900 | 1.00 | 23.62 | C |
| ATOM | 788 | C | GLU | A | 110 | -1.249 | -0.135 | 13.300 | 1.00 | 23.88 | C |
| ATOM | 789 | O | GLU | A | 110 | -2.188 | -0.296 | 12.519 | 1.00 | 24.16 | O |
| ATOM | 790 | CB | GLU | A | 110 | 0.978 | -0.097 | 12.125 | 1.00 | 23.71 | C |
| ATOM | 791 | CG | GLU | A | 110 | 0.663 | -0.221 | 10.640 | 1.00 | 24.25 | C |
| ATOM | 792 | CD | GLU | A | 110 | 1.781 | -0.859 | 9.837 | 1.00 | 24.51 | C |
| ATOM | 793 | OE1 | GLU | A | 110 | 1.796 | -2.101 | 9.716 | 1.00 | 25.02 | O |
| ATOM | 794 | OE2 | GLU | A | 110 | 2.636 | -0.120 | 9.308 | 1.00 | 24.74 | O |
| ATOM | 795 | N | HIS | A | 111 | -1.211 | -0.686 | 14.513 | 1.00 | 24.14 | N |
| ATOM | 796 | CA | HIS | A | 111 | -2.284 | -1.555 | 15.009 | 1.00 | 24.29 | C |
| ATOM | 797 | C | HIS | A | 111 | -3.073 | -0.928 | 16.169 | 1.00 | 24.39 | C |
| ATOM | 798 | O | HIS | A | 111 | -3.360 | -1.589 | 17.172 | 1.00 | 24.14 | O |
| ATOM | 799 | CB | HIS | A | 111 | -1.725 | -2.927 | 15.406 | 1.00 | 24.23 | C |
| ATOM | 800 | CG | HIS | A | 111 | -1.061 | -3.658 | 14.281 | 1.00 | 24.34 | C |
| ATOM | 801 | ND1 | HIS | A | 111 | 0.307 | -3.801 | 14.191 | 1.00 | 24.43 | N |
| ATOM | 802 | CE1 | HIS | A | 111 | 0.605 | -4.483 | 13.099 | 1.00 | 24.21 | C |
| ATOM | 803 | NE2 | HIS | A | 111 | -0.519 | -4.787 | 12.478 | 1.00 | 24.25 | N |
| ATOM | 804 | CD2 | HIS | A | 111 | -1.577 | -4.284 | 13.196 | 1.00 | 24.27 | C |
| ATOM | 805 | N | LYS | A | 112 | -3.423 | 0.349 | 16.014 | 1.00 | 24.75 | N |
| ATOM | 806 | CA | LYS | A | 112 | -4.198 | 1.087 | 17.014 | 1.00 | 25.07 | C |
| ATOM | 807 | C | LYS | A | 112 | -5.543 | 0.413 | 17.301 | 1.00 | 25.32 | C |
| ATOM | 808 | O | LYS | A | 112 | -6.367 | 0.235 | 16.395 | 1.00 | 25.54 | O |
| ATOM | 809 | CB | LYS | A | 112 | -4.419 | 2.533 | 16.565 | 1.00 | 24.93 | C |
| ATOM | 810 | CG | LYS | A | 112 | -3.216 | 3.434 | 16.762 | 1.00 | 25.39 | C |
| ATOM | 811 | CD | LYS | A | 112 | -3.415 | 4.786 | 16.093 | 1.00 | 25.76 | C |
| ATOM | 812 | CE | LYS | A | 112 | -2.172 | 5.652 | 16.216 | 1.00 | 25.95 | C |
| ATOM | 813 | NZ | LYS | A | 112 | -2.035 | 6.247 | 17.578 | 1.00 | 26.44 | N |
| ATOM | 814 | N | ASP | A | 113 | -5.739 | 0.035 | 18.564 | 1.00 | 25.33 | N |
| ATOM | 815 | CA | ASP | A | 113 | -6.950 | -0.651 | 19.028 | 1.00 | 25.33 | C |
| ATOM | 816 | C | ASP | A | 113 | -7.201 | -1.987 | 18.312 | 1.00 | 25.23 | C |
| ATOM | 817 | O | ASP | A | 113 | -8.350 | -2.384 | 18.093 | 1.00 | 25.58 | O |
| ATOM | 818 | CB | ASP | A | 113 | -8.173 | 0.276 | 18.940 | 1.00 | 25.39 | C |
| ATOM | 819 | N | ASN | A | 114 | -6.113 | -2.671 | 17.960 | 1.00 | 24.90 | N |
| ATOM | 820 | CA | ASN | A | 114 | -6.171 | -3.981 | 17.314 | 1.00 | 24.46 | C |
| ATOM | 821 | C | ASN | A | 114 | -5.196 | -4.980 | 17.950 | 1.00 | 24.25 | C |
| ATOM | 822 | O | ASN | A | 114 | -5.069 | -6.119 | 17.500 | 1.00 | 24.20 | O |
| ATOM | 823 | CB | ASN | A | 114 | -5.912 | -3.847 | 15.810 | 1.00 | 24.64 | C |
| ATOM | 824 | CG | ASN | A | 114 | -6.504 | -4.993 | 15.008 | 1.00 | 24.41 | C |
| ATOM | 825 | OD1 | ASN | A | 114 | -7.719 | -5.201 | 14.996 | 1.00 | 24.43 | O |
| ATOM | 826 | ND2 | ASN | A | 114 | -5.643 | -5.743 | 14.330 | 1.00 | 24.11 | N |
| ATOM | 827 | N | ILE | A | 115 | -4.505 | -4.533 | 18.995 | 1.00 | 24.08 | N |
| ATOM | 828 | CA | ILE | A | 115 | -3.672 | -5.405 | 19.818 | 1.00 | 23.73 | C |
| ATOM | 829 | C | ILE | A | 115 | -4.448 | -5.786 | 21.078 | 1.00 | 23.47 | C |
| ATOM | 830 | O | ILE | A | 115 | -5.055 | -4.929 | 21.725 | 1.00 | 23.56 | O |
| ATOM | 831 | CB | ILE | A | 115 | -2.343 | -4.708 | 20.193 | 1.00 | 23.74 | C |
| ATOM | 832 | CG1 | ILE | A | 115 | -1.615 | -4.209 | 18.941 | 1.00 | 23.87 | C |
| ATOM | 833 | CD1 | ILE | A | 115 | -0.899 | -2.891 | 19.135 | 1.00 | 23.85 | C |
| ATOM | 834 | CG2 | ILE | A | 115 | -1.441 | -5.653 | 20.983 | 1.00 | 23.98 | C |
| ATOM | 835 | N | GLY | A | 116 | -4.429 | -7.073 | 21.415 | 1.00 | 22.94 | N |

FIG. 4N

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 836 | CA | GLY | A | 116 | -5.103 | -7.573 | 22.599 | 1.00 | 22.60 | C |
| ATOM | 837 | C | GLY | A | 116 | -4.396 | -7.208 | 23.892 | 1.00 | 22.40 | C |
| ATOM | 838 | O | GLY | A | 116 | -3.251 | -6.747 | 23.878 | 1.00 | 22.38 | O |
| ATOM | 839 | N | SER | A | 117 | -5.088 | -7.422 | 25.009 | 1.00 | 22.12 | N |
| ATOM | 840 | CA | SER | A | 117 | -4.558 | -7.114 | 26.339 | 1.00 | 21.83 | C |
| ATOM | 841 | C | SER | A | 117 | -3.441 | -8.064 | 26.751 | 1.00 | 21.57 | C |
| ATOM | 842 | O | SER | A | 117 | -2.580 | -7.702 | 27.555 | 1.00 | 21.49 | O |
| ATOM | 843 | CB | SER | A | 117 | -5.676 | -7.138 | 27.390 | 1.00 | 21.91 | C |
| ATOM | 844 | OG | SER | A | 117 | -6.555 | -8.235 | 27.193 | 1.00 | 21.91 | O |
| ATOM | 845 | N | GLN | A | 118 | -3.465 | -9.276 | 26.201 | 1.00 | 21.34 | N |
| ATOM | 846 | CA | GLN | A | 118 | -2.458 | -10.287 | 26.503 | 1.00 | 21.12 | C |
| ATOM | 847 | C | GLN | A | 118 | -1.077 | -9.861 | 26.002 | 1.00 | 21.11 | C |
| ATOM | 848 | O | GLN | A | 118 | -0.097 | -9.964 | 26.733 | 1.00 | 20.98 | O |
| ATOM | 849 | CB | GLN | A | 118 | -2.864 | -11.650 | 25.925 | 1.00 | 20.93 | C |
| ATOM | 850 | CG | GLN | A | 118 | -1.952 | -12.816 | 26.314 | 1.00 | 21.00 | C |
| ATOM | 851 | CD | GLN | A | 118 | -1.973 | -13.123 | 27.805 | 1.00 | 20.93 | C |
| ATOM | 852 | OE1 | GLN | A | 118 | -1.174 | -12.577 | 28.568 | 1.00 | 21.15 | O |
| ATOM | 853 | NE2 | GLN | A | 118 | -2.881 | -13.997 | 28.219 | 1.00 | 20.38 | N |
| ATOM | 854 | N | TYR | A | 119 | -1.018 | -9.368 | 24.766 | 1.00 | 21.15 | N |
| ATOM | 855 | CA | TYR | A | 119 | 0.232 | -8.915 | 24.156 | 1.00 | 21.24 | C |
| ATOM | 856 | C | TYR | A | 119 | 0.756 | -7.623 | 24.783 | 1.00 | 21.05 | C |
| ATOM | 857 | O | TYR | A | 119 | 1.967 | -7.455 | 24.936 | 1.00 | 20.83 | O |
| ATOM | 858 | CB | TYR | A | 119 | 0.060 | -8.735 | 22.643 | 1.00 | 21.58 | C |
| ATOM | 859 | CG | TYR | A | 119 | 0.053 | -10.033 | 21.872 | 1.00 | 22.24 | C |
| ATOM | 860 | CD1 | TYR | A | 119 | 1.206 | -10.498 | 21.246 | 1.00 | 22.59 | C |
| ATOM | 861 | CE1 | TYR | A | 119 | 1.206 | -11.698 | 20.537 | 1.00 | 23.26 | C |
| ATOM | 862 | CZ | TYR | A | 119 | 0.040 | -12.441 | 20.453 | 1.00 | 23.55 | C |
| ATOM | 863 | OH | TYR | A | 119 | 0.031 | -13.629 | 19.757 | 1.00 | 24.38 | O |
| ATOM | 864 | CE2 | TYR | A | 119 | -1.120 | -11.998 | 21.067 | 1.00 | 23.26 | C |
| ATOM | 865 | CD2 | TYR | A | 119 | -1.110 | -10.800 | 21.770 | 1.00 | 22.85 | C |
| ATOM | 866 | N | LEU | A | 120 | -0.158 | -6.721 | 25.140 | 1.00 | 20.87 | N |
| ATOM | 867 | CA | LEU | A | 120 | 0.202 | -5.445 | 25.759 | 1.00 | 20.64 | C |
| ATOM | 868 | C | LEU | A | 120 | 0.861 | -5.637 | 27.121 | 1.00 | 20.48 | C |
| ATOM | 869 | O | LEU | A | 120 | 1.908 | -5.046 | 27.397 | 1.00 | 20.68 | O |
| ATOM | 870 | CB | LEU | A | 120 | -1.022 | -4.533 | 25.896 | 1.00 | 20.53 | C |
| ATOM | 871 | CG | LEU | A | 120 | -1.410 | -3.673 | 24.690 | 1.00 | 20.55 | C |
| ATOM | 872 | CD1 | LEU | A | 120 | -2.808 | -3.095 | 24.882 | 1.00 | 20.39 | C |
| ATOM | 873 | CD2 | LEU | A | 120 | -0.393 | -2.563 | 24.434 | 1.00 | 20.42 | C |
| ATOM | 874 | N | LEU | A | 121 | 0.248 | -6.469 | 27.960 | 1.00 | 19.98 | N |
| ATOM | 875 | CA | LEU | A | 121 | 0.778 | -6.746 | 29.293 | 1.00 | 19.62 | C |
| ATOM | 876 | C | LEU | A | 121 | 2.035 | -7.613 | 29.242 | 1.00 | 19.36 | C |
| ATOM | 877 | O | LEU | A | 121 | 2.931 | -7.460 | 30.076 | 1.00 | 19.37 | O |
| ATOM | 878 | CB | LEU | A | 121 | -0.290 | -7.386 | 30.186 | 1.00 | 19.64 | C |
| ATOM | 879 | CG | LEU | A | 121 | -1.394 | -6.440 | 30.667 | 1.00 | 19.34 | C |
| ATOM | 880 | CD1 | LEU | A | 121 | -2.681 | -7.200 | 30.946 | 1.00 | 18.84 | C |
| ATOM | 881 | CD2 | LEU | A | 121 | -0.955 | -5.646 | 31.887 | 1.00 | 19.08 | C |
| ATOM | 882 | N | ASN | A | 122 | 2.094 | -8.512 | 28.260 | 1.00 | 18.94 | N |
| ATOM | 883 | CA | ASN | A | 122 | 3.278 | -9.332 | 28.014 | 1.00 | 18.57 | C |
| ATOM | 884 | C | ASN | A | 122 | 4.501 | -8.479 | 27.681 | 1.00 | 18.33 | C |
| ATOM | 885 | O | ASN | A | 122 | 5.601 | -8.749 | 28.167 | 1.00 | 18.13 | O |
| ATOM | 886 | CB | ASN | A | 122 | 3.019 | -10.332 | 26.882 | 1.00 | 18.68 | C |
| ATOM | 887 | CG | ASN | A | 122 | 2.368 | -11.624 | 27.364 | 1.00 | 18.94 | C |
| ATOM | 888 | OD1 | ASN | A | 122 | 2.342 | -12.618 | 26.639 | 1.00 | 19.98 | O |
| ATOM | 889 | ND2 | ASN | A | 122 | 1.828 | -11.611 | 28.576 | 1.00 | 18.77 | N |
| ATOM | 890 | N | TRP | A | 123 | 4.294 | -7.447 | 26.861 | 1.00 | 18.03 | N |
| ATOM | 891 | CA | TRP | A | 123 | 5.358 | -6.516 | 26.482 | 1.00 | 17.83 | C |
| ATOM | 892 | C | TRP | A | 123 | 5.942 | -5.801 | 27.703 | 1.00 | 17.55 | C |
| ATOM | 893 | O | TRP | A | 123 | 7.167 | -5.709 | 27.846 | 1.00 | 17.38 | O |
| ATOM | 894 | CB | TRP | A | 123 | 4.860 | -5.507 | 25.436 | 1.00 | 17.78 | C |
| ATOM | 895 | CG | TRP | A | 123 | 4.534 | -6.123 | 24.092 | 1.00 | 18.02 | C |

FIG. 40

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 896 | CD1 | TRP | A | 123 | 5.027 | -7.295 | 23.579 | 1.00 | 18.24 | C |
| ATOM | 897 | NE1 | TRP | A | 123 | 4.499 | -7.529 | 22.331 | 1.00 | 18.13 | N |
| ATOM | 898 | CE2 | TRP | A | 123 | 3.642 | -6.509 | 22.011 | 1.00 | 17.96 | C |
| ATOM | 899 | CD2 | TRP | A | 123 | 3.639 | -5.603 | 23.098 | 1.00 | 18.22 | C |
| ATOM | 900 | CE3 | TRP | A | 123 | 2.831 | -4.458 | 23.011 | 1.00 | 18.14 | C |
| ATOM | 901 | CZ3 | TRP | A | 123 | 2.069 | -4.257 | 21.864 | 1.00 | 17.77 | C |
| ATOM | 902 | CH2 | TRP | A | 123 | 2.100 | -5.177 | 20.804 | 1.00 | 18.00 | C |
| ATOM | 903 | CZ2 | TRP | A | 123 | 2.877 | -6.306 | 20.859 | 1.00 | 17.93 | C |
| ATOM | 904 | N | CYS | A | 124 | 5.062 | -5.323 | 28.585 | 1.00 | 17.03 | N |
| ATOM | 905 | CA | CYS | A | 124 | 5.471 | -4.704 | 29.847 | 1.00 | 16.59 | C |
| ATOM | 906 | C | CYS | A | 124 | 6.273 | -5.674 | 30.718 | 1.00 | 16.58 | C |
| ATOM | 907 | O | CYS | A | 124 | 7.219 | -5.262 | 31.394 | 1.00 | 16.52 | O |
| ATOM | 908 | CB | CYS | A | 124 | 4.257 | -4.175 | 30.617 | 1.00 | 16.60 | C |
| ATOM | 909 | SG | CYS | A | 124 | 3.203 | -3.031 | 29.689 | 1.00 | 15.92 | S |
| ATOM | 910 | N | VAL | A | 125 | 5.896 | -6.956 | 30.693 | 1.00 | 16.20 | N |
| ATOM | 911 | CA | VAL | A | 125 | 6.645 | -8.005 | 31.388 | 1.00 | 15.83 | C |
| ATOM | 912 | C | VAL | A | 125 | 8.038 | -8.155 | 30.773 | 1.00 | 15.49 | C |
| ATOM | 913 | O | VAL | A | 125 | 9.040 | -8.194 | 31.491 | 1.00 | 15.37 | O |
| ATOM | 914 | CB | VAL | A | 125 | 5.918 | -9.386 | 31.349 | 1.00 | 15.89 | C |
| ATOM | 915 | CG1 | VAL | A | 125 | 6.772 | -10.476 | 31.989 | 1.00 | 15.63 | C |
| ATOM | 916 | CG2 | VAL | A | 125 | 4.573 | -9.320 | 32.036 | 1.00 | 16.05 | C |
| ATOM | 917 | N | GLN | A | 126 | 8.087 | -8.228 | 29.444 | 1.00 | 15.03 | N |
| ATOM | 918 | CA | GLN | A | 126 | 9.329 | -8.499 | 28.722 | 1.00 | 14.63 | C |
| ATOM | 919 | C | GLN | A | 126 | 10.327 | -7.345 | 28.800 | 1.00 | 14.22 | C |
| ATOM | 920 | O | GLN | A | 126 | 11.527 | -7.572 | 28.907 | 1.00 | 14.18 | O |
| ATOM | 921 | CB | GLN | A | 126 | 9.041 | -8.886 | 27.267 | 1.00 | 14.73 | C |
| ATOM | 922 | CG | GLN | A | 126 | 8.420 | -10.273 | 27.113 | 1.00 | 14.70 | C |
| ATOM | 923 | CD | GLN | A | 126 | 8.163 | -10.676 | 25.667 | 1.00 | 15.18 | C |
| ATOM | 924 | OE1 | GLN | A | 126 | 8.143 | -9.839 | 24.771 | 1.00 | 15.11 | O |
| ATOM | 925 | NE2 | GLN | A | 126 | 7.957 | -11.970 | 25.445 | 1.00 | 16.09 | N |
| ATOM | 926 | N | ILE | A | 127 | 9.827 | -6.112 | 28.761 | 1.00 | 14.17 | N |
| ATOM | 927 | CA | ILE | A | 127 | 10.682 | -4.931 | 28.897 | 1.00 | 13.74 | C |
| ATOM | 928 | C | ILE | A | 127 | 11.219 | -4.811 | 30.329 | 1.00 | 13.55 | C |
| ATOM | 929 | O | ILE | A | 127 | 12.400 | -4.510 | 30.529 | 1.00 | 13.38 | O |
| ATOM | 930 | CB | ILE | A | 127 | 9.947 | -3.642 | 28.437 | 1.00 | 13.70 | C |
| ATOM | 931 | CG1 | ILE | A | 127 | 9.651 | -3.704 | 26.936 | 1.00 | 13.47 | C |
| ATOM | 932 | CD1 | ILE | A | 127 | 8.417 | -2.941 | 26.507 | 1.00 | 13.43 | C |
| ATOM | 933 | CG2 | ILE | A | 127 | 10.777 | -2.395 | 28.749 | 1.00 | 14.06 | C |
| ATOM | 934 | N | ALA | A | 128 | 10.360 | -5.069 | 31.315 | 1.00 | 13.26 | N |
| ATOM | 935 | CA | ALA | A | 128 | 10.782 | -5.073 | 32.717 | 1.00 | 13.19 | C |
| ATOM | 936 | C | ALA | A | 128 | 11.834 | -6.150 | 32.984 | 1.00 | 13.12 | C |
| ATOM | 937 | O | ALA | A | 128 | 12.792 | -5.915 | 33.717 | 1.00 | 12.89 | O |
| ATOM | 938 | CB | ALA | A | 128 | 9.589 | -5.247 | 33.642 | 1.00 | 13.22 | C |
| ATOM | 939 | N | LYS | A | 129 | 11.646 | -7.321 | 32.375 | 1.00 | 13.39 | N |
| ATOM | 940 | CA | LYS | A | 129 | 12.597 | -8.428 | 32.465 | 1.00 | 13.63 | C |
| ATOM | 941 | C | LYS | A | 129 | 13.982 | -8.029 | 31.962 | 1.00 | 13.65 | C |
| ATOM | 942 | O | LYS | A | 129 | 14.983 | -8.263 | 32.641 | 1.00 | 13.64 | O |
| ATOM | 943 | CB | LYS | A | 129 | 12.090 | -9.633 | 31.670 | 1.00 | 13.64 | C |
| ATOM | 944 | CG | LYS | A | 129 | 11.708 | -10.826 | 32.521 | 1.00 | 14.06 | C |
| ATOM | 945 | CD | LYS | A | 129 | 10.474 | -11.522 | 31.974 | 1.00 | 14.78 | C |
| ATOM | 946 | CE | LYS | A | 129 | 10.846 | -12.768 | 31.189 | 1.00 | 15.45 | C |
| ATOM | 947 | NZ | LYS | A | 129 | 9.872 | -13.028 | 30.096 | 1.00 | 16.44 | N |
| ATOM | 948 | N | GLY | A | 130 | 14.023 | -7.427 | 30.773 | 1.00 | 13.68 | N |
| ATOM | 949 | CA | GLY | A | 130 | 15.263 | -6.989 | 30.155 | 1.00 | 13.85 | C |
| ATOM | 950 | C | GLY | A | 130 | 15.910 | -5.800 | 30.847 | 1.00 | 13.91 | C |
| ATOM | 951 | O | GLY | A | 130 | 17.134 | -5.673 | 30.850 | 1.00 | 13.92 | O |
| ATOM | 952 | N | MET | A | 131 | 15.086 | -4.924 | 31.421 | 1.00 | 14.05 | N |
| ATOM | 953 | CA | MET | A | 131 | 15.578 | -3.790 | 32.200 | 1.00 | 14.04 | C |
| ATOM | 954 | C | MET | A | 131 | 16.183 | -4.253 | 33.521 | 1.00 | 13.87 | C |
| ATOM | 955 | O | MET | A | 131 | 17.202 | -3.722 | 33.954 | 1.00 | 14.02 | O |

FIG. 4P

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 956 | CB | MET | A | 131 | 14.464 | -2.772 | 32.458 | 1.00 | 14.17 | C |
| ATOM | 957 | CG | MET | A | 131 | 14.115 | -1.875 | 31.268 | 1.00 | 14.47 | C |
| ATOM | 958 | SD | MET | A | 131 | 15.527 | -1.154 | 30.395 | 1.00 | 14.30 | S |
| ATOM | 959 | CE | MET | A | 131 | 16.077 | 0.063 | 31.559 | 1.00 | 14.66 | C |
| ATOM | 960 | N | ASN | A | 132 | 15.557 | -5.248 | 34.149 | 1.00 | 14.00 | N |
| ATOM | 961 | CA | ASN | A | 132 | 16.097 | -5.870 | 35.361 | 1.00 | 14.12 | C |
| ATOM | 962 | C | ASN | A | 132 | 17.455 | -6.520 | 35.126 | 1.00 | 14.16 | C |
| ATOM | 963 | O | ASN | A | 132 | 18.321 | -6.488 | 36.003 | 1.00 | 13.96 | O |
| ATOM | 964 | CB | ASN | A | 132 | 15.118 | -6.895 | 35.943 | 1.00 | 14.01 | C |
| ATOM | 965 | CG | ASN | A | 132 | 15.664 | -7.590 | 37.181 | 1.00 | 13.85 | C |
| ATOM | 966 | OD1 | ASN | A | 132 | 15.927 | -6.950 | 38.195 | 1.00 | 13.94 | O |
| ATOM | 967 | ND2 | ASN | A | 132 | 15.851 | -8.904 | 37.094 | 1.00 | 13.83 | N |
| ATOM | 968 | N | TYR | A | 133 | 17.631 | -7.100 | 33.941 | 1.00 | 14.46 | N |
| ATOM | 969 | CA | TYR | A | 133 | 18.905 | -7.695 | 33.546 | 1.00 | 14.93 | C |
| ATOM | 970 | C | TYR | A | 133 | 20.013 | -6.653 | 33.499 | 1.00 | 15.03 | C |
| ATOM | 971 | O | TYR | A | 133 | 21.098 | -6.870 | 34.041 | 1.00 | 15.09 | O |
| ATOM | 972 | CB | TYR | A | 133 | 18.794 | -8.392 | 32.190 | 1.00 | 14.86 | C |
| ATOM | 973 | CG | TYR | A | 133 | 20.109 | -8.961 | 31.712 | 1.00 | 15.45 | C |
| ATOM | 974 | CD1 | TYR | A | 133 | 20.586 | -10.174 | 32.207 | 1.00 | 15.42 | C |
| ATOM | 975 | CE1 | TYR | A | 133 | 21.798 | -10.697 | 31.777 | 1.00 | 15.95 | C |
| ATOM | 976 | CZ | TYR | A | 133 | 22.551 | -10.005 | 30.844 | 1.00 | 16.11 | C |
| ATOM | 977 | OH | TYR | A | 133 | 23.750 | -10.524 | 30.415 | 1.00 | 16.45 | O |
| ATOM | 978 | CE2 | TYR | A | 133 | 22.105 | -8.793 | 30.343 | 1.00 | 16.01 | C |
| ATOM | 979 | CD2 | TYR | A | 133 | 20.889 | -8.278 | 30.777 | 1.00 | 15.79 | C |
| ATOM | 980 | N | LEU | A | 134 | 19.728 | -5.529 | 32.842 | 1.00 | 15.43 | N |
| ATOM | 981 | CA | LEU | A | 134 | 20.669 | -4.415 | 32.734 | 1.00 | 15.54 | C |
| ATOM | 982 | C | LEU | A | 134 | 21.023 | -3.873 | 34.116 | 1.00 | 15.53 | C |
| ATOM | 983 | O | LEU | A | 134 | 22.183 | -3.563 | 34.384 | 1.00 | 15.60 | O |
| ATOM | 984 | CB | LEU | A | 134 | 20.100 | -3.303 | 31.841 | 1.00 | 15.46 | C |
| ATOM | 985 | CG | LEU | A | 134 | 19.903 | -3.594 | 30.345 | 1.00 | 15.60 | C |
| ATOM | 986 | CD1 | LEU | A | 134 | 19.222 | -2.421 | 29.644 | 1.00 | 15.26 | C |
| ATOM | 987 | CD2 | LEU | A | 134 | 21.213 | -3.952 | 29.638 | 1.00 | 15.39 | C |
| ATOM | 988 | N | GLU | A | 135 | 20.020 | -3.775 | 34.987 | 1.00 | 15.59 | N |
| ATOM | 989 | CA | GLU | A | 135 | 20.238 | -3.406 | 36.384 | 1.00 | 15.71 | C |
| ATOM | 990 | C | GLU | A | 135 | 21.181 | -4.399 | 37.068 | 1.00 | 15.74 | C |
| ATOM | 991 | O | GLU | A | 135 | 22.108 | -3.989 | 37.772 | 1.00 | 15.87 | O |
| ATOM | 992 | CB | GLU | A | 135 | 18.906 | -3.305 | 37.141 | 1.00 | 15.64 | C |
| ATOM | 993 | CG | GLU | A | 135 | 19.044 | -3.244 | 38.658 | 1.00 | 15.90 | C |
| ATOM | 994 | CD | GLU | A | 135 | 18.038 | -2.323 | 39.327 | 1.00 | 16.38 | C |
| ATOM | 995 | OE1 | GLU | A | 135 | 18.386 | -1.738 | 40.371 | 1.00 | 16.68 | O |
| ATOM | 996 | OE2 | GLU | A | 135 | 16.899 | -2.185 | 38.828 | 1.00 | 17.01 | O |
| ATOM | 997 | N | ASP | A | 136 | 20.948 | -5.695 | 36.843 | 1.00 | 15.53 | N |
| ATOM | 998 | CA | ASP | A | 136 | 21.761 | -6.757 | 37.437 | 1.00 | 15.42 | C |
| ATOM | 999 | C | ASP | A | 136 | 23.209 | -6.723 | 36.945 | 1.00 | 15.65 | C |
| ATOM | 1000 | O | ASP | A | 136 | 24.124 | -7.130 | 37.661 | 1.00 | 15.81 | O |
| ATOM | 1001 | CB | ASP | A | 136 | 21.142 | -8.133 | 37.173 | 1.00 | 15.08 | C |
| ATOM | 1002 | CG | ASP | A | 136 | 20.075 | -8.506 | 38.195 | 1.00 | 14.79 | C |
| ATOM | 1003 | OD1 | ASP | A | 136 | 19.203 | -9.333 | 37.857 | 1.00 | 14.50 | O |
| ATOM | 1004 | OD2 | ASP | A | 136 | 20.021 | -8.035 | 39.353 | 1.00 | 13.86 | O |
| ATOM | 1005 | N | ARG | A | 137 | 23.405 | -6.229 | 35.724 | 1.00 | 15.75 | N |
| ATOM | 1006 | CA | ARG | A | 137 | 24.738 | -6.055 | 35.158 | 1.00 | 15.75 | C |
| ATOM | 1007 | C | ARG | A | 137 | 25.296 | -4.665 | 35.479 | 1.00 | 16.06 | C |
| ATOM | 1008 | O | ARG | A | 137 | 26.324 | -4.257 | 34.930 | 1.00 | 16.25 | O |
| ATOM | 1009 | CB | ARG | A | 137 | 24.714 | -6.298 | 33.642 | 1.00 | 15.43 | C |
| ATOM | 1010 | CG | ARG | A | 137 | 24.445 | -7.748 | 33.236 | 1.00 | 15.41 | C |
| ATOM | 1011 | CD | ARG | A | 137 | 25.674 | -8.653 | 33.240 | 1.00 | 15.00 | C |
| ATOM | 1012 | NE | ARG | A | 137 | 26.361 | -8.648 | 31.950 | 1.00 | 15.35 | N |
| ATOM | 1013 | CZ | ARG | A | 137 | 27.624 | -8.270 | 31.767 | 1.00 | 16.00 | C |
| ATOM | 1014 | NH1 | ARG | A | 137 | 28.368 | -7.863 | 32.787 | 1.00 | 16.20 | N |
| ATOM | 1015 | NH2 | ARG | A | 137 | 28.150 | -8.300 | 30.554 | 1.00 | 16.19 | N |

FIG. 4Q

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1016 | N | ARG | A | 138 | 24.610 | -3.953 | 36.377 | 1.00 | 16.30 | N |
| ATOM | 1017 | CA | ARG | A | 138 | 24.972 | -2.591 | 36.795 | 1.00 | 16.39 | C |
| ATOM | 1018 | C | ARG | A | 138 | 25.133 | -1.644 | 35.603 | 1.00 | 16.43 | C |
| ATOM | 1019 | O | ARG | A | 138 | 26.125 | -0.919 | 35.493 | 1.00 | 16.47 | O |
| ATOM | 1020 | CB | ARG | A | 138 | 26.220 | -2.593 | 37.694 | 1.00 | 16.44 | C |
| ATOM | 1021 | CG | ARG | A | 138 | 26.096 | -3.448 | 38.962 | 1.00 | 16.86 | C |
| ATOM | 1022 | CD | ARG | A | 138 | 25.064 | -2.933 | 39.960 | 1.00 | 17.57 | C |
| ATOM | 1023 | NE | ARG | A | 138 | 24.744 | -3.899 | 41.012 | 1.00 | 17.41 | N |
| ATOM | 1024 | CZ | ARG | A | 138 | 23.510 | -4.217 | 41.394 | 1.00 | 17.24 | C |
| ATOM | 1025 | NH1 | ARG | A | 138 | 22.457 | -3.668 | 40.803 | 1.00 | 16.80 | N |
| ATOM | 1026 | NH2 | ARG | A | 138 | 23.326 | -5.096 | 42.371 | 1.00 | 17.60 | N |
| ATOM | 1027 | N | LEU | A | 139 | 24.142 | -1.669 | 34.713 | 1.00 | 16.41 | N |
| ATOM | 1028 | CA | LEU | A | 139 | 24.147 | -0.849 | 33.503 | 1.00 | 16.25 | C |
| ATOM | 1029 | C | LEU | A | 139 | 22.907 | 0.032 | 33.428 | 1.00 | 16.12 | C |
| ATOM | 1030 | O | LEU | A | 139 | 21.777 | -0.466 | 33.401 | 1.00 | 16.11 | O |
| ATOM | 1031 | CB | LEU | A | 139 | 24.232 | -1.727 | 32.249 | 1.00 | 16.18 | C |
| ATOM | 1032 | CG | LEU | A | 139 | 25.393 | -2.719 | 32.103 | 1.00 | 16.35 | C |
| ATOM | 1033 | CD1 | LEU | A | 139 | 25.139 | -3.640 | 30.920 | 1.00 | 16.00 | C |
| ATOM | 1034 | CD2 | LEU | A | 139 | 26.739 | -2.003 | 31.956 | 1.00 | 16.32 | C |
| ATOM | 1035 | N | VAL | A | 140 | 23.127 | 1.343 | 33.406 | 1.00 | 15.91 | N |
| ATOM | 1036 | CA | VAL | A | 140 | 22.040 | 2.305 | 33.255 | 1.00 | 15.76 | C |
| ATOM | 1037 | C | VAL | A | 140 | 21.759 | 2.479 | 31.765 | 1.00 | 15.77 | C |
| ATOM | 1038 | O | VAL | A | 140 | 22.687 | 2.597 | 30.965 | 1.00 | 16.09 | O |
| ATOM | 1039 | CB | VAL | A | 140 | 22.373 | 3.659 | 33.931 | 1.00 | 15.73 | C |
| ATOM | 1040 | CG1 | VAL | A | 140 | 21.219 | 4.655 | 33.782 | 1.00 | 15.53 | C |
| ATOM | 1041 | CG2 | VAL | A | 140 | 22.706 | 3.451 | 35.408 | 1.00 | 15.49 | C |
| ATOM | 1042 | N | HIS | A | 141 | 20.481 | 2.466 | 31.398 | 1.00 | 15.61 | N |
| ATOM | 1043 | CA | HIS | A | 141 | 20.083 | 2.592 | 29.999 | 1.00 | 15.51 | C |
| ATOM | 1044 | C | HIS | A | 141 | 20.237 | 4.021 | 29.485 | 1.00 | 15.35 | C |
| ATOM | 1045 | O | HIS | A | 141 | 20.917 | 4.249 | 28.483 | 1.00 | 15.17 | O |
| ATOM | 1046 | CB | HIS | A | 141 | 18.648 | 2.099 | 29.786 | 1.00 | 15.44 | C |
| ATOM | 1047 | CG | HIS | A | 141 | 18.279 | 1.941 | 28.345 | 1.00 | 15.37 | C |
| ATOM | 1048 | ND1 | HIS | A | 141 | 18.061 | 0.711 | 27.764 | 1.00 | 15.41 | N |
| ATOM | 1049 | CE1 | HIS | A | 141 | 17.766 | 0.879 | 26.486 | 1.00 | 15.73 | C |
| ATOM | 1050 | NE2 | HIS | A | 141 | 17.786 | 2.172 | 26.218 | 1.00 | 15.30 | N |
| ATOM | 1051 | CD2 | HIS | A | 141 | 18.109 | 2.858 | 27.363 | 1.00 | 15.35 | C |
| ATOM | 1052 | N | ARG | A | 142 | 19.577 | 4.966 | 30.159 | 1.00 | 15.30 | N |
| ATOM | 1053 | CA | ARG | A | 142 | 19.722 | 6.399 | 29.885 | 1.00 | 15.16 | C |
| ATOM | 1054 | C | ARG | A | 142 | 18.887 | 6.934 | 28.711 | 1.00 | 14.70 | C |
| ATOM | 1055 | O | ARG | A | 142 | 18.870 | 8.145 | 28.468 | 1.00 | 14.69 | O |
| ATOM | 1056 | CB | ARG | A | 142 | 21.199 | 6.749 | 29.680 | 1.00 | 15.59 | C |
| ATOM | 1057 | CG | ARG | A | 142 | 21.635 | 8.016 | 30.338 | 1.00 | 16.40 | C |
| ATOM | 1058 | CD | ARG | A | 142 | 23.099 | 8.312 | 30.154 | 1.00 | 18.03 | C |
| ATOM | 1059 | NE | ARG | A | 142 | 23.907 | 7.603 | 31.138 | 1.00 | 19.00 | N |
| ATOM | 1060 | CZ | ARG | A | 142 | 24.785 | 8.185 | 31.940 | 1.00 | 19.30 | C |
| ATOM | 1061 | NH1 | ARG | A | 142 | 24.980 | 9.495 | 31.878 | 1.00 | 19.43 | N |
| ATOM | 1062 | NH2 | ARG | A | 142 | 25.471 | 7.454 | 32.808 | 1.00 | 19.76 | N |
| ATOM | 1063 | N | ASP | A | 143 | 18.198 | 6.042 | 27.997 | 1.00 | 13.94 | N |
| ATOM | 1064 | CA | ASP | A | 143 | 17.387 | 6.430 | 26.837 | 1.00 | 13.35 | C |
| ATOM | 1065 | C | ASP | A | 143 | 16.296 | 5.402 | 26.491 | 1.00 | 13.04 | C |
| ATOM | 1066 | O | ASP | A | 143 | 16.093 | 5.060 | 25.323 | 1.00 | 12.50 | O |
| ATOM | 1067 | CB | ASP | A | 143 | 18.292 | 6.691 | 25.623 | 1.00 | 13.48 | C |
| ATOM | 1068 | CG | ASP | A | 143 | 17.555 | 7.329 | 24.455 | 1.00 | 13.74 | C |
| ATOM | 1069 | OD1 | ASP | A | 143 | 16.493 | 7.965 | 24.657 | 1.00 | 13.89 | O |
| ATOM | 1070 | OD2 | ASP | A | 143 | 17.975 | 7.239 | 23.287 | 1.00 | 13.81 | O |
| ATOM | 1071 | N | LEU | A | 144 | 15.596 | 4.911 | 27.510 | 1.00 | 12.63 | N |
| ATOM | 1072 | CA | LEU | A | 144 | 14.526 | 3.949 | 27.286 | 1.00 | 12.23 | C |
| ATOM | 1073 | C | LEU | A | 144 | 13.273 | 4.650 | 26.767 | 1.00 | 12.03 | C |
| ATOM | 1074 | O | LEU | A | 144 | 12.858 | 5.688 | 27.293 | 1.00 | 11.80 | O |
| ATOM | 1075 | CB | LEU | A | 144 | 14.227 | 3.128 | 28.549 | 1.00 | 12.33 | C |

FIG. 4R

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 1076 | CG | LEU | A | 144 | 13.240 | 1.955 | 28.416 | 1.00 | 12.30 | C |
| ATOM | 1077 | CD1 | LEU | A | 144 | 13.783 | 0.833 | 27.522 | 1.00 | 11.94 | C |
| ATOM | 1078 | CD2 | LEU | A | 144 | 12.867 | 1.415 | 29.784 | 1.00 | 12.32 | C |
| ATOM | 1079 | N | ALA | A | 145 | 12.698 | 4.063 | 25.721 | 1.00 | 11.66 | N |
| ATOM | 1080 | CA | ALA | A | 145 | 11.527 | 4.589 | 25.030 | 1.00 | 11.54 | C |
| ATOM | 1081 | C | ALA | A | 145 | 10.880 | 3.441 | 24.266 | 1.00 | 11.51 | C |
| ATOM | 1082 | O | ALA | A | 145 | 11.500 | 2.385 | 24.093 | 1.00 | 11.58 | O |
| ATOM | 1083 | CB | ALA | A | 145 | 11.934 | 5.705 | 24.070 | 1.00 | 11.25 | C |
| ATOM | 1084 | N | ALA | A | 146 | 9.643 | 3.637 | 23.809 | 1.00 | 11.22 | N |
| ATOM | 1085 | CA | ALA | A | 146 | 8.981 | 2.635 | 22.974 | 1.00 | 11.36 | C |
| ATOM | 1086 | C | ALA | A | 146 | 9.666 | 2.531 | 21.612 | 1.00 | 11.56 | C |
| ATOM | 1087 | O | ALA | A | 146 | 9.609 | 1.485 | 20.955 | 1.00 | 11.93 | O |
| ATOM | 1088 | CB | ALA | A | 146 | 7.502 | 2.942 | 22.816 | 1.00 | 11.16 | C |
| ATOM | 1089 | N | ARG | A | 147 | 10.317 | 3.619 | 21.203 | 1.00 | 11.49 | N |
| ATOM | 1090 | CA | ARG | A | 147 | 11.093 | 3.644 | 19.968 | 1.00 | 11.56 | C |
| ATOM | 1091 | C | ARG | A | 147 | 12.376 | 2.819 | 20.100 | 1.00 | 12.09 | C |
| ATOM | 1092 | O | ARG | A | 147 | 12.922 | 2.354 | 19.099 | 1.00 | 12.37 | O |
| ATOM | 1093 | CB | ARG | A | 147 | 11.402 | 5.090 | 19.534 | 1.00 | 11.01 | C |
| ATOM | 1094 | CG | ARG | A | 147 | 12.485 | 5.802 | 20.341 | 1.00 | 9.48 | C |
| ATOM | 1095 | CD | ARG | A | 147 | 12.519 | 7.316 | 20.171 | 1.00 | 7.47 | C |
| ATOM | 1096 | NE | ARG | A | 147 | 13.431 | 7.949 | 21.123 | 1.00 | 5.04 | N |
| ATOM | 1097 | CZ | ARG | A | 147 | 13.052 | 8.633 | 22.202 | 1.00 | 5.82 | C |
| ATOM | 1098 | NH1 | ARG | A | 147 | 11.765 | 8.791 | 22.483 | 1.00 | 5.76 | N |
| ATOM | 1099 | NH2 | ARG | A | 147 | 13.965 | 9.165 | 23.008 | 1.00 | 5.16 | N |
| ATOM | 1100 | N | ASN | A | 148 | 12.846 | 2.641 | 21.333 | 1.00 | 12.61 | N |
| ATOM | 1101 | CA | ASN | A | 148 | 14.078 | 1.897 | 21.590 | 1.00 | 13.19 | C |
| ATOM | 1102 | C | ASN | A | 148 | 13.822 | 0.468 | 22.070 | 1.00 | 13.54 | C |
| ATOM | 1103 | O | ASN | A | 148 | 14.684 | -0.164 | 22.680 | 1.00 | 13.69 | O |
| ATOM | 1104 | CB | ASN | A | 148 | 14.989 | 2.671 | 22.550 | 1.00 | 13.15 | C |
| ATOM | 1105 | CG | ASN | A | 148 | 15.726 | 3.813 | 21.861 | 1.00 | 13.53 | C |
| ATOM | 1106 | OD1 | ASN | A | 148 | 15.887 | 3.816 | 20.640 | 1.00 | 13.84 | O |
| ATOM | 1107 | ND2 | ASN | A | 148 | 16.176 | 4.790 | 22.644 | 1.00 | 13.47 | N |
| ATOM | 1108 | N | VAL | A | 149 | 12.620 | -0.025 | 21.787 | 1.00 | 14.09 | N |
| ATOM | 1109 | CA | VAL | A | 149 | 12.273 | -1.429 | 21.973 | 1.00 | 14.37 | C |
| ATOM | 1110 | C | VAL | A | 149 | 11.944 | -1.994 | 20.597 | 1.00 | 14.62 | C |
| ATOM | 1111 | O | VAL | A | 149 | 11.054 | -1.483 | 19.910 | 1.00 | 14.75 | O |
| ATOM | 1112 | CB | VAL | A | 149 | 11.064 | -1.612 | 22.922 | 1.00 | 14.42 | C |
| ATOM | 1113 | CG1 | VAL | A | 149 | 10.720 | -3.089 | 23.082 | 1.00 | 14.46 | C |
| ATOM | 1114 | CG2 | VAL | A | 149 | 11.335 | -0.981 | 24.281 | 1.00 | 14.24 | C |
| ATOM | 1115 | N | LEU | A | 150 | 12.667 | -3.036 | 20.195 | 1.00 | 14.74 | N |
| ATOM | 1116 | CA | LEU | A | 150 | 12.506 | -3.622 | 18.866 | 1.00 | 14.99 | C |
| ATOM | 1117 | C | LEU | A | 150 | 11.660 | -4.894 | 18.875 | 1.00 | 15.26 | C |
| ATOM | 1118 | O | LEU | A | 150 | 11.748 | -5.709 | 19.795 | 1.00 | 15.33 | O |
| ATOM | 1119 | CB | LEU | A | 150 | 13.872 | -3.900 | 18.225 | 1.00 | 15.05 | C |
| ATOM | 1120 | CG | LEU | A | 150 | 14.788 | -2.723 | 17.865 | 1.00 | 15.07 | C |
| ATOM | 1121 | CD1 | LEU | A | 150 | 16.191 | -3.229 | 17.582 | 1.00 | 15.01 | C |
| ATOM | 1122 | CD2 | LEU | A | 150 | 14.261 | -1.924 | 16.673 | 1.00 | 15.24 | C |
| ATOM | 1123 | N | VAL | A | 151 | 10.856 | -5.059 | 17.827 | 1.00 | 15.71 | N |
| ATOM | 1124 | CA | VAL | A | 151 | 9.973 | -6.213 | 17.680 | 1.00 | 16.00 | C |
| ATOM | 1125 | C | VAL | A | 151 | 10.694 | -7.394 | 17.025 | 1.00 | 16.38 | C |
| ATOM | 1126 | O | VAL | A | 151 | 10.889 | -7.408 | 15.809 | 1.00 | 16.66 | O |
| ATOM | 1127 | CB | VAL | A | 151 | 8.708 | -5.856 | 16.849 | 1.00 | 15.94 | C |
| ATOM | 1128 | CG1 | VAL | A | 151 | 7.722 | -7.018 | 16.821 | 1.00 | 15.70 | C |
| ATOM | 1129 | CG2 | VAL | A | 151 | 8.035 | -4.600 | 17.389 | 1.00 | 15.48 | C |
| ATOM | 1130 | N | LYS | A | 152 | 11.087 | -8.377 | 17.834 | 1.00 | 16.71 | N |
| ATOM | 1131 | CA | LYS | A | 152 | 11.634 | -9.631 | 17.313 | 1.00 | 17.11 | C |
| ATOM | 1132 | C | LYS | A | 152 | 10.521 | -10.398 | 16.607 | 1.00 | 17.51 | C |
| ATOM | 1133 | O | LYS | A | 152 | 10.658 | -10.773 | 15.438 | 1.00 | 17.61 | O |
| ATOM | 1134 | CB | LYS | A | 152 | 12.246 | -10.476 | 18.437 | 1.00 | 17.15 | C |
| ATOM | 1135 | CG | LYS | A | 152 | 13.295 | -11.482 | 17.975 | 1.00 | 16.68 | C |

FIG. 4S

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 1136 | N | THR | A | 153 | 9.431 | -10.631 | 17.341 | 1.00 | 17.88 | N |
| ATOM | 1137 | CA | THR | A | 153 | 8.164 | -11.139 | 16.806 | 1.00 | 18.19 | C |
| ATOM | 1138 | C | THR | A | 153 | 7.038 | -10.433 | 17.570 | 1.00 | 18.52 | C |
| ATOM | 1139 | O | THR | A | 153 | 7.300 | -9.834 | 18.615 | 1.00 | 18.53 | O |
| ATOM | 1140 | CB | THR | A | 153 | 8.037 | -12.685 | 16.981 | 1.00 | 18.12 | C |
| ATOM | 1141 | OG1 | THR | A | 153 | 7.904 | -13.012 | 18.371 | 1.00 | 18.04 | O |
| ATOM | 1142 | CG2 | THR | A | 153 | 9.307 | -13.423 | 16.553 | 1.00 | 18.27 | C |
| ATOM | 1143 | N | PRO | A | 154 | 5.795 | -10.493 | 17.082 | 1.00 | 18.87 | N |
| ATOM | 1144 | CA | PRO | A | 154 | 4.659 | -9.917 | 17.818 | 1.00 | 19.12 | C |
| ATOM | 1145 | C | PRO | A | 154 | 4.620 | -10.297 | 19.307 | 1.00 | 19.43 | C |
| ATOM | 1146 | O | PRO | A | 154 | 4.094 | -9.530 | 20.114 | 1.00 | 19.21 | O |
| ATOM | 1147 | CB | PRO | A | 154 | 3.447 | -10.499 | 17.089 | 1.00 | 19.02 | C |
| ATOM | 1148 | CG | PRO | A | 154 | 3.913 | -10.688 | 15.702 | 1.00 | 18.89 | C |
| ATOM | 1149 | CD | PRO | A | 154 | 5.364 | -11.076 | 15.796 | 1.00 | 18.96 | C |
| ATOM | 1150 | N | GLN | A | 155 | 5.182 | -11.452 | 19.659 | 1.00 | 19.97 | N |
| ATOM | 1151 | CA | GLN | A | 155 | 5.165 | -11.932 | 21.043 | 1.00 | 20.54 | C |
| ATOM | 1152 | C | GLN | A | 155 | 6.540 | -11.902 | 21.728 | 1.00 | 20.48 | C |
| ATOM | 1153 | O | GLN | A | 155 | 6.698 | -12.395 | 22.849 | 1.00 | 20.38 | O |
| ATOM | 1154 | CB | GLN | A | 155 | 4.531 | -13.333 | 21.131 | 1.00 | 20.84 | C |
| ATOM | 1155 | CG | GLN | A | 155 | 5.085 | -14.375 | 20.160 | 1.00 | 21.92 | C |
| ATOM | 1156 | CD | GLN | A | 155 | 4.441 | -14.315 | 18.777 | 1.00 | 23.72 | C |
| ATOM | 1157 | OE1 | GLN | A | 155 | 5.141 | -14.391 | 17.760 | 1.00 | 24.36 | O |
| ATOM | 1158 | NE2 | GLN | A | 155 | 3.114 | -14.177 | 18.735 | 1.00 | 23.67 | N |
| ATOM | 1159 | N | HIS | A | 156 | 7.522 | -11.303 | 21.057 | 1.00 | 20.46 | N |
| ATOM | 1160 | CA | HIS | A | 156 | 8.882 | -11.203 | 21.582 | 1.00 | 20.45 | C |
| ATOM | 1161 | C | HIS | A | 156 | 9.462 | -9.819 | 21.287 | 1.00 | 20.43 | C |
| ATOM | 1162 | O | HIS | A | 156 | 9.701 | -9.478 | 20.130 | 1.00 | 20.54 | O |
| ATOM | 1163 | CB | HIS | A | 156 | 9.757 | -12.299 | 20.963 | 1.00 | 20.35 | C |
| ATOM | 1164 | CG | HIS | A | 156 | 11.064 | -12.512 | 21.661 | 1.00 | 20.28 | C |
| ATOM | 1165 | ND1 | HIS | A | 156 | 11.423 | -13.726 | 22.208 | 1.00 | 20.15 | N |
| ATOM | 1166 | CE1 | HIS | A | 156 | 12.625 | -13.626 | 22.747 | 1.00 | 19.81 | C |
| ATOM | 1167 | NE2 | HIS | A | 156 | 13.062 | -12.393 | 22.563 | 1.00 | 19.97 | N |
| ATOM | 1168 | CD2 | HIS | A | 156 | 12.107 | -11.678 | 21.882 | 1.00 | 20.26 | C |
| ATOM | 1169 | N | VAL | A | 157 | 9.675 | -9.026 | 22.335 | 1.00 | 20.36 | N |
| ATOM | 1170 | CA | VAL | A | 157 | 10.275 | -7.695 | 22.191 | 1.00 | 20.44 | C |
| ATOM | 1171 | C | VAL | A | 157 | 11.646 | -7.604 | 22.868 | 1.00 | 20.70 | C |
| ATOM | 1172 | O | VAL | A | 157 | 11.932 | -8.330 | 23.826 | 1.00 | 20.82 | O |
| ATOM | 1173 | CB | VAL | A | 157 | 9.347 | -6.553 | 22.703 | 1.00 | 20.38 | C |
| ATOM | 1174 | CG1 | VAL | A | 157 | 8.062 | -6.494 | 21.892 | 1.00 | 20.44 | C |
| ATOM | 1175 | CG2 | VAL | A | 157 | 9.050 | -6.686 | 24.201 | 1.00 | 20.11 | C |
| ATOM | 1176 | N | LYS | A | 158 | 12.488 | -6.706 | 22.361 | 1.00 | 20.85 | N |
| ATOM | 1177 | CA | LYS | A | 158 | 13.846 | -6.545 | 22.872 | 1.00 | 20.92 | C |
| ATOM | 1178 | C | LYS | A | 158 | 14.212 | -5.077 | 23.021 | 1.00 | 20.94 | C |
| ATOM | 1179 | O | LYS | A | 158 | 13.925 | -4.268 | 22.140 | 1.00 | 21.23 | O |
| ATOM | 1180 | CB | LYS | A | 158 | 14.852 | -7.217 | 21.935 | 1.00 | 21.03 | C |
| ATOM | 1181 | CG | LYS | A | 158 | 14.901 | -8.735 | 22.032 | 1.00 | 21.12 | C |
| ATOM | 1182 | CD | LYS | A | 158 | 15.345 | -9.358 | 20.717 | 1.00 | 21.17 | C |
| ATOM | 1183 | CE | LYS | A | 158 | 16.860 | -9.469 | 20.639 | 1.00 | 21.47 | C |
| ATOM | 1184 | NZ | LYS | A | 158 | 17.364 | -10.713 | 21.279 | 1.00 | 21.60 | N |
| ATOM | 1185 | N | ILE | A | 159 | 14.854 | -4.747 | 24.137 | 1.00 | 20.82 | N |
| ATOM | 1186 | CA | ILE | A | 159 | 15.380 | -3.406 | 24.373 | 1.00 | 20.62 | C |
| ATOM | 1187 | C | ILE | A | 159 | 16.663 | -3.190 | 23.565 | 1.00 | 20.60 | C |
| ATOM | 1188 | O | ILE | A | 159 | 17.511 | -4.083 | 23.477 | 1.00 | 20.36 | O |
| ATOM | 1189 | CB | ILE | A | 159 | 15.651 | -3.196 | 25.883 | 1.00 | 20.67 | C |
| ATOM | 1190 | CG1 | ILE | A | 159 | 14.357 | -3.319 | 26.690 | 1.00 | 20.75 | C |
| ATOM | 1191 | CD1 | ILE | A | 159 | 14.558 | -3.910 | 28.064 | 1.00 | 20.51 | C |
| ATOM | 1192 | CG2 | ILE | A | 159 | 16.291 | -1.846 | 26.142 | 1.00 | 20.48 | C |
| ATOM | 1193 | N | THR | A | 160 | 16.792 | -2.001 | 22.980 | 1.00 | 20.67 | N |
| ATOM | 1194 | CA | THR | A | 160 | 17.994 | -1.618 | 22.237 | 1.00 | 20.69 | C |
| ATOM | 1195 | C | THR | A | 160 | 18.545 | -0.252 | 22.681 | 1.00 | 20.96 | C |

FIG. 4T

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1196 | O | THR | A | 160 | 17.920 | 0.442 | 23.487 | 1.00 | 20.89 | O |
| ATOM | 1197 | CB | THR | A | 160 | 17.726 | -1.674 | 20.704 | 1.00 | 20.50 | C |
| ATOM | 1198 | OG1 | THR | A | 160 | 18.952 | -1.493 | 19.988 | 1.00 | 20.44 | O |
| ATOM | 1199 | CG2 | THR | A | 160 | 16.859 | -0.510 | 20.237 | 1.00 | 20.18 | C |
| ATOM | 1200 | N | ASP | A | 161 | 19.723 | 0.103 | 22.164 | 1.00 | 21.46 | N |
| ATOM | 1201 | CA | ASP | A | 161 | 20.374 | 1.404 | 22.395 | 1.00 | 22.05 | C |
| ATOM | 1202 | C | ASP | A | 161 | 20.705 | 1.735 | 23.855 | 1.00 | 22.41 | C |
| ATOM | 1203 | O | ASP | A | 161 | 20.660 | 2.899 | 24.266 | 1.00 | 22.54 | O |
| ATOM | 1204 | CB | ASP | A | 161 | 19.568 | 2.554 | 21.769 | 1.00 | 22.09 | C |
| ATOM | 1205 | CG | ASP | A | 161 | 19.421 | 2.427 | 20.265 | 1.00 | 22.27 | C |
| ATOM | 1206 | OD1 | ASP | A | 161 | 20.299 | 1.828 | 19.601 | 1.00 | 22.13 | O |
| ATOM | 1207 | OD2 | ASP | A | 161 | 18.448 | 2.917 | 19.659 | 1.00 | 22.54 | O |
| ATOM | 1208 | N | PHE | A | 162 | 21.048 | 0.715 | 24.633 | 1.00 | 22.90 | N |
| ATOM | 1209 | CA | PHE | A | 162 | 21.460 | 0.926 | 26.018 | 1.00 | 23.38 | C |
| ATOM | 1210 | C | PHE | A | 162 | 22.930 | 1.343 | 26.094 | 1.00 | 23.35 | C |
| ATOM | 1211 | O | PHE | A | 162 | 23.759 | 0.877 | 25.308 | 1.00 | 23.15 | O |
| ATOM | 1212 | CB | PHE | A | 162 | 21.210 | -0.333 | 26.857 | 1.00 | 23.55 | C |
| ATOM | 1213 | CG | PHE | A | 162 | 22.102 | -1.486 | 26.502 | 1.00 | 24.06 | C |
| ATOM | 1214 | CD1 | PHE | A | 162 | 23.276 | -1.717 | 27.214 | 1.00 | 24.57 | C |
| ATOM | 1215 | CE1 | PHE | A | 162 | 24.108 | -2.784 | 26.888 | 1.00 | 25.22 | C |
| ATOM | 1216 | CZ | PHE | A | 162 | 23.766 | -3.634 | 25.835 | 1.00 | 25.31 | C |
| ATOM | 1217 | CE2 | PHE | A | 162 | 22.596 | -3.412 | 25.121 | 1.00 | 25.47 | C |
| ATOM | 1218 | CD2 | PHE | A | 162 | 21.771 | -2.341 | 25.457 | 1.00 | 24.79 | C |
| ATOM | 1219 | N | GLY | A | 163 | 23.234 | 2.228 | 27.041 | 1.00 | 23.34 | N |
| ATOM | 1220 | CA | GLY | A | 163 | 24.598 | 2.643 | 27.317 | 1.00 | 23.63 | C |
| ATOM | 1221 | C | GLY | A | 163 | 25.268 | 3.467 | 26.233 | 1.00 | 23.74 | C |
| ATOM | 1222 | O | GLY | A | 163 | 26.395 | 3.171 | 25.832 | 1.00 | 23.81 | O |
| ATOM | 1223 | N | LEU | A | 164 | 24.573 | 4.497 | 25.758 | 1.00 | 23.77 | N |
| ATOM | 1224 | CA | LEU | A | 164 | 25.152 | 5.456 | 24.824 | 1.00 | 23.85 | C |
| ATOM | 1225 | C | LEU | A | 164 | 25.226 | 6.833 | 25.485 | 1.00 | 24.12 | C |
| ATOM | 1226 | O | LEU | A | 164 | 24.213 | 7.532 | 25.628 | 1.00 | 24.22 | O |
| ATOM | 1227 | CB | LEU | A | 164 | 24.363 | 5.506 | 23.509 | 1.00 | 23.82 | C |
| ATOM | 1228 | CG | LEU | A | 164 | 23.879 | 4.195 | 22.869 | 1.00 | 23.87 | C |
| ATOM | 1229 | CD1 | LEU | A | 164 | 22.887 | 4.480 | 21.757 | 1.00 | 24.37 | C |
| ATOM | 1230 | CD2 | LEU | A | 164 | 25.022 | 3.341 | 22.340 | 1.00 | 24.15 | C |
| ATOM | 1231 | N | ALA | A | 165 | 26.435 | 7.193 | 25.913 | 1.00 | 24.18 | N |
| ATOM | 1232 | CA | ALA | A | 165 | 26.705 | 8.449 | 26.610 | 1.00 | 24.07 | C |
| ATOM | 1233 | C | ALA | A | 165 | 28.210 | 8.711 | 26.643 | 1.00 | 24.11 | C |
| ATOM | 1234 | O | ALA | A | 165 | 29.013 | 7.774 | 26.693 | 1.00 | 23.96 | O |
| ATOM | 1235 | CB | ALA | A | 165 | 26.147 | 8.406 | 28.027 | 1.00 | 24.03 | C |
| ATOM | 1236 | N | VAL | A | 182 | 18.270 | 15.907 | 25.552 | 1.00 | 25.02 | N |
| ATOM | 1237 | CA | VAL | A | 182 | 17.370 | 15.974 | 24.400 | 1.00 | 24.71 | C |
| ATOM | 1238 | C | VAL | A | 182 | 15.981 | 15.360 | 24.686 | 1.00 | 24.32 | C |
| ATOM | 1239 | O | VAL | A | 182 | 14.980 | 16.075 | 24.583 | 1.00 | 24.64 | O |
| ATOM | 1240 | CB | VAL | A | 182 | 18.017 | 15.386 | 23.101 | 1.00 | 24.93 | C |
| ATOM | 1241 | CG1 | VAL | A | 182 | 17.059 | 15.479 | 21.911 | 1.00 | 25.38 | C |
| ATOM | 1242 | CG2 | VAL | A | 182 | 19.324 | 16.100 | 22.776 | 1.00 | 25.20 | C |
| ATOM | 1243 | N | PRO | A | 183 | 15.905 | 14.072 | 25.056 | 1.00 | 23.64 | N |
| ATOM | 1244 | CA | PRO | A | 183 | 14.607 | 13.407 | 25.248 | 1.00 | 23.03 | C |
| ATOM | 1245 | C | PRO | A | 183 | 13.988 | 13.682 | 26.623 | 1.00 | 22.51 | C |
| ATOM | 1246 | O | PRO | A | 183 | 13.675 | 12.744 | 27.364 | 1.00 | 22.55 | O |
| ATOM | 1247 | CB | PRO | A | 183 | 14.957 | 11.923 | 25.098 | 1.00 | 23.21 | C |
| ATOM | 1248 | CG | PRO | A | 183 | 16.372 | 11.814 | 25.589 | 1.00 | 23.32 | C |
| ATOM | 1249 | CD | PRO | A | 183 | 17.025 | 13.147 | 25.324 | 1.00 | 23.47 | C |
| ATOM | 1250 | N | ILE | A | 184 | 13.801 | 14.964 | 26.933 | 1.00 | 21.88 | N |
| ATOM | 1251 | CA | ILE | A | 184 | 13.321 | 15.430 | 28.241 | 1.00 | 21.08 | C |
| ATOM | 1252 | C | ILE | A | 184 | 12.059 | 14.714 | 28.729 | 1.00 | 20.43 | C |
| ATOM | 1253 | O | ILE | A | 184 | 11.942 | 14.395 | 29.913 | 1.00 | 20.47 | O |
| ATOM | 1254 | CB | ILE | A | 184 | 13.095 | 16.979 | 28.209 | 1.00 | 21.15 | C |
| ATOM | 1255 | CG1 | ILE | A | 184 | 14.378 | 17.717 | 27.798 | 1.00 | 21.07 | C |

FIG. 4U

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1256 | CD1 | ILE | A | 184 | 15.546 | 17.598 | 28.783 | 1.00 | 21.24 | C |
| ATOM | 1257 | CG2 | ILE | A | 184 | 12.542 | 17.506 | 29.547 | 1.00 | 21.12 | C |
| ATOM | 1258 | N | LYS | A | 185 | 11.136 | 14.448 | 27.808 | 1.00 | 19.70 | N |
| ATOM | 1259 | CA | LYS | A | 185 | 9.806 | 13.925 | 28.141 | 1.00 | 18.98 | C |
| ATOM | 1260 | C | LYS | A | 185 | 9.784 | 12.468 | 28.609 | 1.00 | 18.35 | C |
| ATOM | 1261 | O | LYS | A | 185 | 8.745 | 11.964 | 29.043 | 1.00 | 18.25 | O |
| ATOM | 1262 | CB | LYS | A | 185 | 8.858 | 14.117 | 26.955 | 1.00 | 19.09 | C |
| ATOM | 1263 | CG | LYS | A | 185 | 8.452 | 15.565 | 26.742 | 1.00 | 19.08 | C |
| ATOM | 1264 | CD | LYS | A | 185 | 7.699 | 15.744 | 25.449 | 1.00 | 19.02 | C |
| ATOM | 1265 | CE | LYS | A | 185 | 7.606 | 17.206 | 25.089 | 1.00 | 19.14 | C |
| ATOM | 1266 | NZ | LYS | A | 185 | 6.468 | 17.462 | 24.170 | 1.00 | 19.61 | N |
| ATOM | 1267 | N | TRP | A | 186 | 10.929 | 11.799 | 28.515 | 1.00 | 17.68 | N |
| ATOM | 1268 | CA | TRP | A | 186 | 11.071 | 10.424 | 28.975 | 1.00 | 17.10 | C |
| ATOM | 1269 | C | TRP | A | 186 | 11.950 | 10.373 | 30.220 | 1.00 | 17.01 | C |
| ATOM | 1270 | O | TRP | A | 186 | 11.997 | 9.358 | 30.911 | 1.00 | 17.17 | O |
| ATOM | 1271 | CB | TRP | A | 186 | 11.681 | 9.551 | 27.874 | 1.00 | 16.98 | C |
| ATOM | 1272 | CG | TRP | A | 186 | 10.709 | 9.126 | 26.815 | 1.00 | 16.64 | C |
| ATOM | 1273 | CD1 | TRP | A | 186 | 10.019 | 7.945 | 26.759 | 1.00 | 16.55 | C |
| ATOM | 1274 | NE1 | TRP | A | 186 | 9.222 | 7.913 | 25.639 | 1.00 | 16.12 | N |
| ATOM | 1275 | CE2 | TRP | A | 186 | 9.386 | 9.080 | 24.941 | 1.00 | 16.13 | C |
| ATOM | 1276 | CD2 | TRP | A | 186 | 10.321 | 9.869 | 25.652 | 1.00 | 16.26 | C |
| ATOM | 1277 | CE3 | TRP | A | 186 | 10.664 | 11.129 | 25.137 | 1.00 | 16.01 | C |
| ATOM | 1278 | CZ3 | TRP | A | 186 | 10.074 | 11.552 | 23.945 | 1.00 | 15.63 | C |
| ATOM | 1279 | CH2 | TRP | A | 186 | 9.150 | 10.743 | 23.267 | 1.00 | 15.58 | C |
| ATOM | 1280 | CZ2 | TRP | A | 186 | 8.794 | 9.507 | 23.746 | 1.00 | 15.70 | C |
| ATOM | 1281 | N | MET | A | 187 | 12.641 | 11.475 | 30.498 | 1.00 | 16.65 | N |
| ATOM | 1282 | CA | MET | A | 187 | 13.620 | 11.537 | 31.580 | 1.00 | 16.45 | C |
| ATOM | 1283 | C | MET | A | 187 | 13.000 | 11.794 | 32.951 | 1.00 | 16.40 | C |
| ATOM | 1284 | O | MET | A | 187 | 11.997 | 12.504 | 33.072 | 1.00 | 16.38 | O |
| ATOM | 1285 | CB | MET | A | 187 | 14.660 | 12.618 | 31.290 | 1.00 | 16.42 | C |
| ATOM | 1286 | CG | MET | A | 187 | 15.631 | 12.269 | 30.181 | 1.00 | 16.96 | C |
| ATOM | 1287 | SD | MET | A | 187 | 16.550 | 13.704 | 29.610 | 1.00 | 18.00 | S |
| ATOM | 1288 | CE | MET | A | 187 | 17.971 | 12.896 | 28.891 | 1.00 | 18.94 | C |
| ATOM | 1289 | N | ALA | A | 188 | 13.620 | 11.212 | 33.977 | 1.00 | 16.07 | N |
| ATOM | 1290 | CA | ALA | A | 188 | 13.285 | 11.500 | 35.366 | 1.00 | 15.66 | C |
| ATOM | 1291 | C | ALA | A | 188 | 13.661 | 12.942 | 35.702 | 1.00 | 15.57 | C |
| ATOM | 1292 | O | ALA | A | 188 | 14.498 | 13.541 | 35.024 | 1.00 | 15.35 | O |
| ATOM | 1293 | CB | ALA | A | 188 | 13.999 | 10.530 | 36.291 | 1.00 | 15.72 | C |
| ATOM | 1294 | N | LEU | A | 189 | 13.043 | 13.492 | 36.746 | 1.00 | 15.47 | N |
| ATOM | 1295 | CA | LEU | A | 189 | 13.245 | 14.892 | 37.113 | 1.00 | 15.43 | C |
| ATOM | 1296 | C | LEU | A | 189 | 14.690 | 15.206 | 37.509 | 1.00 | 15.41 | C |
| ATOM | 1297 | O | LEU | A | 189 | 15.222 | 16.261 | 37.154 | 1.00 | 15.47 | O |
| ATOM | 1298 | CB | LEU | A | 189 | 12.274 | 15.313 | 38.222 | 1.00 | 15.48 | C |
| ATOM | 1299 | CG | LEU | A | 189 | 12.259 | 16.799 | 38.600 | 1.00 | 15.39 | C |
| ATOM | 1300 | CD1 | LEU | A | 189 | 11.780 | 17.679 | 37.450 | 1.00 | 15.25 | C |
| ATOM | 1301 | CD2 | LEU | A | 189 | 11.414 | 17.018 | 39.833 | 1.00 | 15.13 | C |
| ATOM | 1302 | N | GLU | A | 190 | 15.320 | 14.282 | 38.227 | 1.00 | 15.32 | N |
| ATOM | 1303 | CA | GLU | A | 190 | 16.716 | 14.434 | 38.628 | 1.00 | 15.39 | C |
| ATOM | 1304 | C | GLU | A | 190 | 17.683 | 14.332 | 37.438 | 1.00 | 15.34 | C |
| ATOM | 1305 | O | GLU | A | 190 | 18.820 | 14.784 | 37.524 | 1.00 | 15.47 | O |
| ATOM | 1306 | CB | GLU | A | 190 | 17.076 | 13.434 | 39.738 | 1.00 | 15.32 | C |
| ATOM | 1307 | CG | GLU | A | 190 | 17.325 | 12.007 | 39.264 | 1.00 | 15.72 | C |
| ATOM | 1308 | CD | GLU | A | 190 | 16.093 | 11.123 | 39.314 | 1.00 | 15.81 | C |
| ATOM | 1309 | OE1 | GLU | A | 190 | 16.259 | 9.883 | 39.274 | 1.00 | 16.54 | O |
| ATOM | 1310 | OE2 | GLU | A | 190 | 14.963 | 11.651 | 39.390 | 1.00 | 15.33 | O |
| ATOM | 1311 | N | SER | A | 191 | 17.221 | 13.743 | 36.336 | 1.00 | 15.30 | N |
| ATOM | 1312 | CA | SER | A | 191 | 18.011 | 13.653 | 35.111 | 1.00 | 15.37 | C |
| ATOM | 1313 | C | SER | A | 191 | 17.987 | 14.961 | 34.328 | 1.00 | 15.40 | C |
| ATOM | 1314 | O | SER | A | 191 | 18.936 | 15.278 | 33.613 | 1.00 | 15.60 | O |
| ATOM | 1315 | CB | SER | A | 191 | 17.508 | 12.512 | 34.223 | 1.00 | 15.43 | C |

FIG. 4V

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1316 | OG | SER | A | 191 | 17.990 | 11.258 | 34.673 | 1.00 | 15.35 | O |
| ATOM | 1317 | N | ILE | A | 192 | 16.897 | 15.712 | 34.465 | 1.00 | 15.50 | N |
| ATOM | 1318 | CA | ILE | A | 192 | 16.714 | 16.974 | 33.745 | 1.00 | 15.42 | C |
| ATOM | 1319 | C | ILE | A | 192 | 17.385 | 18.142 | 34.469 | 1.00 | 15.48 | C |
| ATOM | 1320 | O | ILE | A | 192 | 17.906 | 19.058 | 33.830 | 1.00 | 15.40 | O |
| ATOM | 1321 | CB | ILE | A | 192 | 15.205 | 17.269 | 33.531 | 1.00 | 15.35 | C |
| ATOM | 1322 | CG1 | ILE | A | 192 | 14.527 | 16.114 | 32.790 | 1.00 | 14.87 | C |
| ATOM | 1323 | CD1 | ILE | A | 192 | 13.058 | 15.962 | 33.108 | 1.00 | 15.07 | C |
| ATOM | 1324 | CG2 | ILE | A | 192 | 15.003 | 18.584 | 32.773 | 1.00 | 15.22 | C |
| ATOM | 1325 | N | LEU | A | 193 | 17.368 | 18.100 | 35.799 | 1.00 | 15.57 | N |
| ATOM | 1326 | CA | LEU | A | 193 | 17.897 | 19.194 | 36.611 | 1.00 | 15.62 | C |
| ATOM | 1327 | C | LEU | A | 193 | 19.318 | 18.948 | 37.117 | 1.00 | 15.80 | C |
| ATOM | 1328 | O | LEU | A | 193 | 20.109 | 19.883 | 37.237 | 1.00 | 15.79 | O |
| ATOM | 1329 | CB | LEU | A | 193 | 16.964 | 19.494 | 37.789 | 1.00 | 15.41 | C |
| ATOM | 1330 | CG | LEU | A | 193 | 15.460 | 19.644 | 37.532 | 1.00 | 15.29 | C |
| ATOM | 1331 | CD1 | LEU | A | 193 | 14.715 | 19.684 | 38.856 | 1.00 | 14.80 | C |
| ATOM | 1332 | CD2 | LEU | A | 193 | 15.127 | 20.876 | 36.684 | 1.00 | 14.79 | C |
| ATOM | 1333 | N | HIS | A | 194 | 19.637 | 17.692 | 37.415 | 1.00 | 16.06 | N |
| ATOM | 1334 | CA | HIS | A | 194 | 20.931 | 17.359 | 38.007 | 1.00 | 16.44 | C |
| ATOM | 1335 | C | HIS | A | 194 | 21.814 | 16.561 | 37.057 | 1.00 | 16.42 | C |
| ATOM | 1336 | O | HIS | A | 194 | 23.015 | 16.423 | 37.290 | 1.00 | 16.51 | O |
| ATOM | 1337 | CB | HIS | A | 194 | 20.753 | 16.589 | 39.325 | 1.00 | 16.44 | C |
| ATOM | 1338 | CG | HIS | A | 194 | 19.846 | 17.259 | 40.313 | 1.00 | 16.71 | C |
| ATOM | 1339 | ND1 | HIS | A | 194 | 19.198 | 16.565 | 41.312 | 1.00 | 16.78 | N |
| ATOM | 1340 | CE1 | HIS | A | 194 | 18.471 | 17.404 | 42.028 | 1.00 | 16.92 | C |
| ATOM | 1341 | NE2 | HIS | A | 194 | 18.627 | 18.618 | 41.534 | 1.00 | 17.02 | N |
| ATOM | 1342 | CD2 | HIS | A | 194 | 19.485 | 18.557 | 40.463 | 1.00 | 16.68 | C |
| ATOM | 1343 | N | ARG | A | 195 | 21.209 | 16.047 | 35.987 | 1.00 | 16.63 | N |
| ATOM | 1344 | CA | ARG | A | 195 | 21.875 | 15.142 | 35.048 | 1.00 | 16.70 | C |
| ATOM | 1345 | C | ARG | A | 195 | 22.338 | 13.858 | 35.745 | 1.00 | 16.67 | C |
| ATOM | 1346 | O | ARG | A | 195 | 23.431 | 13.349 | 35.479 | 1.00 | 16.82 | O |
| ATOM | 1347 | CB | ARG | A | 195 | 23.040 | 15.841 | 34.331 | 1.00 | 17.00 | C |
| ATOM | 1348 | CG | ARG | A | 195 | 22.645 | 17.073 | 33.533 | 1.00 | 17.15 | C |
| ATOM | 1349 | CD | ARG | A | 195 | 23.749 | 17.597 | 32.635 | 1.00 | 18.04 | C |
| ATOM | 1350 | NE | ARG | A | 195 | 23.459 | 18.939 | 32.135 | 1.00 | 18.55 | N |
| ATOM | 1351 | CZ | ARG | A | 195 | 24.374 | 19.790 | 31.682 | 1.00 | 18.89 | C |
| ATOM | 1352 | NH1 | ARG | A | 195 | 24.002 | 20.990 | 31.253 | 1.00 | 19.08 | N |
| ATOM | 1353 | NH2 | ARG | A | 195 | 25.659 | 19.451 | 31.655 | 1.00 | 18.55 | N |
| ATOM | 1354 | N | ILE | A | 196 | 21.494 | 13.350 | 36.642 | 1.00 | 16.52 | N |
| ATOM | 1355 | CA | ILE | A | 196 | 21.760 | 12.109 | 37.365 | 1.00 | 16.40 | C |
| ATOM | 1356 | C | ILE | A | 196 | 21.037 | 10.941 | 36.688 | 1.00 | 16.40 | C |
| ATOM | 1357 | O | ILE | A | 196 | 19.845 | 11.036 | 36.374 | 1.00 | 16.50 | O |
| ATOM | 1358 | CB | ILE | A | 196 | 21.337 | 12.250 | 38.850 | 1.00 | 16.44 | C |
| ATOM | 1359 | CG1 | ILE | A | 196 | 22.331 | 13.144 | 39.602 | 1.00 | 16.56 | C |
| ATOM | 1360 | CD1 | ILE | A | 196 | 21.887 | 13.546 | 41.005 | 1.00 | 17.00 | C |
| ATOM | 1361 | CG2 | ILE | A | 196 | 21.213 | 10.877 | 39.525 | 1.00 | 16.41 | C |
| ATOM | 1362 | N | TYR | A | 197 | 21.764 | 9.847 | 36.463 | 1.00 | 16.06 | N |
| ATOM | 1363 | CA | TYR | A | 197 | 21.202 | 8.665 | 35.818 | 1.00 | 15.94 | C |
| ATOM | 1364 | C | TYR | A | 197 | 21.468 | 7.388 | 36.609 | 1.00 | 15.95 | C |
| ATOM | 1365 | O | TYR | A | 197 | 22.607 | 6.919 | 36.691 | 1.00 | 16.09 | O |
| ATOM | 1366 | CB | TYR | A | 197 | 21.737 | 8.524 | 34.393 | 1.00 | 15.99 | C |
| ATOM | 1367 | CG | TYR | A | 197 | 21.366 | 9.667 | 33.478 | 1.00 | 16.10 | C |
| ATOM | 1368 | CD1 | TYR | A | 197 | 20.149 | 9.671 | 32.795 | 1.00 | 16.35 | C |
| ATOM | 1369 | CE1 | TYR | A | 197 | 19.806 | 10.720 | 31.944 | 1.00 | 16.43 | C |
| ATOM | 1370 | CZ | TYR | A | 197 | 20.687 | 11.776 | 31.777 | 1.00 | 16.45 | C |
| ATOM | 1371 | OH | TYR | A | 197 | 20.354 | 12.814 | 30.947 | 1.00 | 17.09 | O |
| ATOM | 1372 | CE2 | TYR | A | 197 | 21.899 | 11.796 | 32.446 | 1.00 | 16.39 | C |
| ATOM | 1373 | CD2 | TYR | A | 197 | 22.232 | 10.744 | 33.292 | 1.00 | 16.30 | C |
| ATOM | 1374 | N | THR | A | 198 | 20.407 | 6.836 | 37.194 | 1.00 | 15.84 | N |
| ATOM | 1375 | CA | THR | A | 198 | 20.496 | 5.592 | 37.956 | 1.00 | 15.92 | C |

FIG. 4W

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1376 | C | THR | A | 198 | 19.527 | 4.554 | 37.388 | 1.00 | 16.16 | C |
| ATOM | 1377 | O | THR | A | 198 | 18.961 | 4.750 | 36.310 | 1.00 | 16.34 | O |
| ATOM | 1378 | CB | THR | A | 198 | 20.221 | 5.833 | 39.467 | 1.00 | 15.89 | C |
| ATOM | 1379 | OG1 | THR | A | 198 | 18.904 | 6.370 | 39.643 | 1.00 | 16.16 | O |
| ATOM | 1380 | CG2 | THR | A | 198 | 21.138 | 6.919 | 40.036 | 1.00 | 15.36 | C |
| ATOM | 1381 | N | HIS | A | 199 | 19.344 | 3.448 | 38.105 | 1.00 | 16.11 | N |
| ATOM | 1382 | CA | HIS | A | 199 | 18.382 | 2.430 | 37.694 | 1.00 | 16.10 | C |
| ATOM | 1383 | C | HIS | A | 199 | 16.950 | 2.884 | 37.976 | 1.00 | 15.96 | C |
| ATOM | 1384 | O | HIS | A | 199 | 16.007 | 2.427 | 37.328 | 1.00 | 16.01 | O |
| ATOM | 1385 | CB | HIS | A | 199 | 18.685 | 1.089 | 38.368 | 1.00 | 16.16 | C |
| ATOM | 1386 | CG | HIS | A | 199 | 20.016 | 0.514 | 37.995 | 1.00 | 16.30 | C |
| ATOM | 1387 | ND1 | HIS | A | 199 | 21.010 | 0.274 | 38.919 | 1.00 | 16.50 | N |
| ATOM | 1388 | CE1 | HIS | A | 199 | 22.068 | -0.229 | 38.307 | 1.00 | 16.31 | C |
| ATOM | 1389 | NE2 | HIS | A | 199 | 21.797 | -0.321 | 37.017 | 1.00 | 16.44 | N |
| ATOM | 1390 | CD2 | HIS | A | 199 | 20.522 | 0.140 | 36.796 | 1.00 | 16.43 | C |
| ATOM | 1391 | N | GLN | A | 200 | 16.803 | 3.794 | 38.940 | 1.00 | 15.71 | N |
| ATOM | 1392 | CA | GLN | A | 200 | 15.511 | 4.398 | 39.266 | 1.00 | 15.24 | C |
| ATOM | 1393 | C | GLN | A | 200 | 15.136 | 5.503 | 38.277 | 1.00 | 14.88 | C |
| ATOM | 1394 | O | GLN | A | 200 | 13.955 | 5.817 | 38.101 | 1.00 | 14.65 | O |
| ATOM | 1395 | CB | GLN | A | 200 | 15.508 | 4.931 | 40.701 | 1.00 | 15.07 | C |
| ATOM | 1396 | CG | GLN | A | 200 | 15.663 | 3.852 | 41.776 | 1.00 | 15.30 | C |
| ATOM | 1397 | CD | GLN | A | 200 | 14.678 | 2.704 | 41.621 | 1.00 | 15.16 | C |
| ATOM | 1398 | OE1 | GLN | A | 200 | 15.028 | 1.652 | 41.091 | 1.00 | 15.03 | O |
| ATOM | 1399 | NE2 | GLN | A | 200 | 13.447 | 2.904 | 42.082 | 1.00 | 15.34 | N |
| ATOM | 1400 | N | SER | A | 201 | 16.147 | 6.087 | 37.640 | 1.00 | 14.65 | N |
| ATOM | 1401 | CA | SER | A | 201 | 15.943 | 7.005 | 36.520 | 1.00 | 14.61 | C |
| ATOM | 1402 | C | SER | A | 201 | 15.288 | 6.270 | 35.351 | 1.00 | 14.26 | C |
| ATOM | 1403 | O | SER | A | 201 | 14.387 | 6.805 | 34.704 | 1.00 | 14.07 | O |
| ATOM | 1404 | CB | SER | A | 201 | 17.278 | 7.598 | 36.063 | 1.00 | 14.61 | C |
| ATOM | 1405 | OG | SER | A | 201 | 17.368 | 8.967 | 36.397 | 1.00 | 15.71 | O |
| ATOM | 1406 | N | ASP | A | 202 | 15.756 | 5.045 | 35.096 | 1.00 | 13.85 | N |
| ATOM | 1407 | CA | ASP | A | 202 | 15.247 | 4.200 | 34.018 | 1.00 | 13.46 | C |
| ATOM | 1408 | C | ASP | A | 202 | 13.810 | 3.751 | 34.273 | 1.00 | 13.21 | C |
| ATOM | 1409 | O | ASP | A | 202 | 13.037 | 3.587 | 33.328 | 1.00 | 13.50 | O |
| ATOM | 1410 | CB | ASP | A | 202 | 16.142 | 2.968 | 33.826 | 1.00 | 13.60 | C |
| ATOM | 1411 | CG | ASP | A | 202 | 17.440 | 3.281 | 33.091 | 1.00 | 13.51 | C |
| ATOM | 1412 | OD1 | ASP | A | 202 | 18.416 | 2.520 | 33.276 | 1.00 | 13.11 | O |
| ATOM | 1413 | OD2 | ASP | A | 202 | 17.584 | 4.249 | 32.311 | 1.00 | 13.33 | O |
| ATOM | 1414 | N | VAL | A | 203 | 13.461 | 3.546 | 35.544 | 1.00 | 12.65 | N |
| ATOM | 1415 | CA | VAL | A | 203 | 12.096 | 3.173 | 35.928 | 1.00 | 12.05 | C |
| ATOM | 1416 | C | VAL | A | 203 | 11.087 | 4.230 | 35.460 | 1.00 | 11.80 | C |
| ATOM | 1417 | O | VAL | A | 203 | 10.033 | 3.887 | 34.918 | 1.00 | 11.87 | O |
| ATOM | 1418 | CB | VAL | A | 203 | 11.967 | 2.907 | 37.460 | 1.00 | 11.93 | C |
| ATOM | 1419 | CG1 | VAL | A | 203 | 10.507 | 2.757 | 37.875 | 1.00 | 11.84 | C |
| ATOM | 1420 | CG2 | VAL | A | 203 | 12.738 | 1.656 | 37.857 | 1.00 | 11.42 | C |
| ATOM | 1421 | N | TRP | A | 204 | 11.427 | 5.504 | 35.658 | 1.00 | 11.36 | N |
| ATOM | 1422 | CA | TRP | A | 204 | 10.624 | 6.625 | 35.165 | 1.00 | 11.08 | C |
| ATOM | 1423 | C | TRP | A | 204 | 10.350 | 6.487 | 33.668 | 1.00 | 10.86 | C |
| ATOM | 1424 | O | TRP | A | 204 | 9.193 | 6.504 | 33.246 | 1.00 | 10.60 | O |
| ATOM | 1425 | CB | TRP | A | 204 | 11.321 | 7.959 | 35.461 | 1.00 | 11.08 | C |
| ATOM | 1426 | CG | TRP | A | 204 | 10.499 | 9.187 | 35.142 | 1.00 | 11.50 | C |
| ATOM | 1427 | CD1 | TRP | A | 204 | 10.020 | 9.567 | 33.918 | 1.00 | 11.52 | C |
| ATOM | 1428 | NE1 | TRP | A | 204 | 9.323 | 10.746 | 34.025 | 1.00 | 11.48 | N |
| ATOM | 1429 | CE2 | TRP | A | 204 | 9.346 | 11.162 | 35.329 | 1.00 | 11.15 | C |
| ATOM | 1430 | CD2 | TRP | A | 204 | 10.079 | 10.204 | 36.063 | 1.00 | 11.66 | C |
| ATOM | 1431 | CE3 | TRP | A | 204 | 10.248 | 10.405 | 37.442 | 1.00 | 11.70 | C |
| ATOM | 1432 | CZ3 | TRP | A | 204 | 9.692 | 11.529 | 38.028 | 1.00 | 11.60 | C |
| ATOM | 1433 | CH2 | TRP | A | 204 | 8.967 | 12.459 | 37.268 | 1.00 | 11.90 | C |
| ATOM | 1434 | CZ2 | TRP | A | 204 | 8.785 | 12.293 | 35.920 | 1.00 | 11.61 | C |
| ATOM | 1435 | N | SER | A | 205 | 11.417 | 6.339 | 32.883 | 1.00 | 10.60 | N |

FIG. 4X

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1436 | CA | SER | A | 205 | 11.319 | 6.168 | 31.432 | 1.00 | 10.78 | C |
| ATOM | 1437 | C | SER | A | 205 | 10.478 | 4.958 | 31.037 | 1.00 | 10.87 | C |
| ATOM | 1438 | O | SER | A | 205 | 9.708 | 5.024 | 30.076 | 1.00 | 10.84 | O |
| ATOM | 1439 | CB | SER | A | 205 | 12.709 | 6.074 | 30.807 | 1.00 | 10.83 | C |
| ATOM | 1440 | OG | SER | A | 205 | 13.424 | 7.284 | 30.992 | 1.00 | 10.86 | O |
| ATOM | 1441 | N | TYR | A | 206 | 10.631 | 3.866 | 31.787 | 1.00 | 11.00 | N |
| ATOM | 1442 | CA | TYR | A | 206 | 9.801 | 2.674 | 31.637 | 1.00 | 11.09 | C |
| ATOM | 1443 | C | TYR | A | 206 | 8.319 | 3.019 | 31.810 | 1.00 | 11.36 | C |
| ATOM | 1444 | O | TYR | A | 206 | 7.483 | 2.582 | 31.020 | 1.00 | 11.57 | O |
| ATOM | 1445 | CB | TYR | A | 206 | 10.245 | 1.594 | 32.633 | 1.00 | 11.20 | C |
| ATOM | 1446 | CG | TYR | A | 206 | 9.383 | 0.347 | 32.673 | 1.00 | 10.90 | C |
| ATOM | 1447 | CD1 | TYR | A | 206 | 8.330 | 0.236 | 33.579 | 1.00 | 11.02 | C |
| ATOM | 1448 | CE1 | TYR | A | 206 | 7.535 | -0.910 | 33.627 | 1.00 | 11.16 | C |
| ATOM | 1449 | CZ | TYR | A | 206 | 7.802 | -1.964 | 32.772 | 1.00 | 10.74 | C |
| ATOM | 1450 | OH | TYR | A | 206 | 7.016 | -3.086 | 32.830 | 1.00 | 10.40 | O |
| ATOM | 1451 | CE2 | TYR | A | 206 | 8.849 | -1.886 | 31.863 | 1.00 | 10.78 | C |
| ATOM | 1452 | CD2 | TYR | A | 206 | 9.635 | -0.731 | 31.821 | 1.00 | 11.05 | C |
| ATOM | 1453 | N | GLY | A | 207 | 8.003 | 3.811 | 32.834 | 1.00 | 11.29 | N |
| ATOM | 1454 | CA | GLY | A | 207 | 6.649 | 4.296 | 33.047 | 1.00 | 11.28 | C |
| ATOM | 1455 | C | GLY | A | 207 | 6.083 | 5.045 | 31.851 | 1.00 | 11.14 | C |
| ATOM | 1456 | O | GLY | A | 207 | 4.928 | 4.847 | 31.476 | 1.00 | 11.25 | O |
| ATOM | 1457 | N | VAL | A | 208 | 6.904 | 5.904 | 31.253 | 1.00 | 11.19 | N |
| ATOM | 1458 | CA | VAL | A | 208 | 6.533 | 6.653 | 30.050 | 1.00 | 11.14 | C |
| ATOM | 1459 | C | VAL | A | 208 | 6.389 | 5.721 | 28.839 | 1.00 | 11.08 | C |
| ATOM | 1460 | O | VAL | A | 208 | 5.473 | 5.884 | 28.030 | 1.00 | 11.10 | O |
| ATOM | 1461 | CB | VAL | A | 208 | 7.555 | 7.782 | 29.747 | 1.00 | 11.13 | C |
| ATOM | 1462 | CG1 | VAL | A | 208 | 7.124 | 8.606 | 28.544 | 1.00 | 11.24 | C |
| ATOM | 1463 | CG2 | VAL | A | 208 | 7.737 | 8.685 | 30.966 | 1.00 | 10.97 | C |
| ATOM | 1464 | N | THR | A | 209 | 7.294 | 4.746 | 28.736 | 1.00 | 10.89 | N |
| ATOM | 1465 | CA | THR | A | 209 | 7.265 | 3.735 | 27.679 | 1.00 | 10.48 | C |
| ATOM | 1466 | C | THR | A | 209 | 5.965 | 2.929 | 27.707 | 1.00 | 10.72 | C |
| ATOM | 1467 | O | THR | A | 209 | 5.346 | 2.711 | 26.664 | 1.00 | 10.81 | O |
| ATOM | 1468 | CB | THR | A | 209 | 8.490 | 2.801 | 27.804 | 1.00 | 10.40 | C |
| ATOM | 1469 | OG1 | THR | A | 209 | 9.691 | 3.570 | 27.675 | 1.00 | 9.30 | O |
| ATOM | 1470 | CG2 | THR | A | 209 | 8.560 | 1.821 | 26.636 | 1.00 | 9.93 | C |
| ATOM | 1471 | N | VAL | A | 210 | 5.560 | 2.497 | 28.902 | 1.00 | 10.80 | N |
| ATOM | 1472 | CA | VAL | A | 210 | 4.296 | 1.788 | 29.099 | 1.00 | 10.97 | C |
| ATOM | 1473 | C | VAL | A | 210 | 3.113 | 2.674 | 28.683 | 1.00 | 11.27 | C |
| ATOM | 1474 | O | VAL | A | 210 | 2.181 | 2.207 | 28.023 | 1.00 | 11.29 | O |
| ATOM | 1475 | CB | VAL | A | 210 | 4.137 | 1.284 | 30.568 | 1.00 | 10.87 | C |
| ATOM | 1476 | CG1 | VAL | A | 210 | 2.769 | 0.644 | 30.794 | 1.00 | 10.41 | C |
| ATOM | 1477 | CG2 | VAL | A | 210 | 5.237 | 0.286 | 30.920 | 1.00 | 11.02 | C |
| ATOM | 1478 | N | TRP | A | 211 | 3.168 | 3.952 | 29.052 | 1.00 | 11.64 | N |
| ATOM | 1479 | CA | TRP | A | 211 | 2.135 | 4.911 | 28.667 | 1.00 | 12.07 | C |
| ATOM | 1480 | C | TRP | A | 211 | 1.984 | 4.992 | 27.149 | 1.00 | 12.36 | C |
| ATOM | 1481 | O | TRP | A | 211 | 0.867 | 5.090 | 26.644 | 1.00 | 12.54 | O |
| ATOM | 1482 | CB | TRP | A | 211 | 2.429 | 6.297 | 29.246 | 1.00 | 12.10 | C |
| ATOM | 1483 | CG | TRP | A | 211 | 1.333 | 7.295 | 29.002 | 1.00 | 12.17 | C |
| ATOM | 1484 | CD1 | TRP | A | 211 | 0.244 | 7.529 | 29.795 | 1.00 | 12.20 | C |
| ATOM | 1485 | NE1 | TRP | A | 211 | -0.540 | 8.516 | 29.245 | 1.00 | 12.12 | N |
| ATOM | 1486 | CE2 | TRP | A | 211 | 0.032 | 8.942 | 28.076 | 1.00 | 11.77 | C |
| ATOM | 1487 | CD2 | TRP | A | 211 | 1.215 | 8.193 | 27.889 | 1.00 | 12.01 | C |
| ATOM | 1488 | CE3 | TRP | A | 211 | 1.992 | 8.442 | 26.746 | 1.00 | 11.94 | C |
| ATOM | 1489 | CZ3 | TRP | A | 211 | 1.568 | 9.416 | 25.844 | 1.00 | 11.61 | C |
| ATOM | 1490 | CH2 | TRP | A | 211 | 0.386 | 10.139 | 26.063 | 1.00 | 11.19 | C |
| ATOM | 1491 | CZ2 | TRP | A | 211 | -0.392 | 9.919 | 27.169 | 1.00 | 11.54 | C |
| ATOM | 1492 | N | GLU | A | 212 | 3.108 | 4.948 | 26.434 | 1.00 | 12.58 | N |
| ATOM | 1493 | CA | GLU | A | 212 | 3.110 | 4.967 | 24.972 | 1.00 | 12.64 | C |
| ATOM | 1494 | C | GLU | A | 212 | 2.363 | 3.768 | 24.399 | 1.00 | 12.97 | C |
| ATOM | 1495 | O | GLU | A | 212 | 1.582 | 3.912 | 23.462 | 1.00 | 13.32 | O |

FIG. 4Y

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1496 | CB | GLU | A | 212 | 4.538 | 4.967 | 24.430 | 1.00 | 12.50 | C |
| ATOM | 1497 | CG | GLU | A | 212 | 5.332 | 6.233 | 24.688 | 1.00 | 11.97 | C |
| ATOM | 1498 | CD | GLU | A | 212 | 6.702 | 6.167 | 24.055 | 1.00 | 11.43 | C |
| ATOM | 1499 | OE1 | GLU | A | 212 | 6.835 | 6.581 | 22.883 | 1.00 | 11.08 | O |
| ATOM | 1500 | OE2 | GLU | A | 212 | 7.641 | 5.680 | 24.722 | 1.00 | 11.03 | O |
| ATOM | 1501 | N | LEU | A | 213 | 2.609 | 2.590 | 24.967 | 1.00 | 13.28 | N |
| ATOM | 1502 | CA | LEU | A | 213 | 1.984 | 1.354 | 24.499 | 1.00 | 13.71 | C |
| ATOM | 1503 | C | LEU | A | 213 | 0.473 | 1.340 | 24.751 | 1.00 | 14.03 | C |
| ATOM | 1504 | O | LEU | A | 213 | -0.310 | 1.016 | 23.852 | 1.00 | 14.12 | O |
| ATOM | 1505 | CB | LEU | A | 213 | 2.652 | 0.129 | 25.140 | 1.00 | 13.65 | C |
| ATOM | 1506 | CG | LEU | A | 213 | 4.172 | -0.042 | 24.981 | 1.00 | 13.61 | C |
| ATOM | 1507 | CD1 | LEU | A | 213 | 4.650 | -1.317 | 25.663 | 1.00 | 13.24 | C |
| ATOM | 1508 | CD2 | LEU | A | 213 | 4.599 | -0.024 | 23.514 | 1.00 | 13.51 | C |
| ATOM | 1509 | N | MET | A | 214 | 0.078 | 1.710 | 25.968 | 1.00 | 14.19 | N |
| ATOM | 1510 | CA | MET | A | 214 | -1.322 | 1.705 | 26.382 | 1.00 | 14.41 | C |
| ATOM | 1511 | C | MET | A | 214 | -2.155 | 2.757 | 25.651 | 1.00 | 14.65 | C |
| ATOM | 1512 | O | MET | A | 214 | -3.373 | 2.606 | 25.526 | 1.00 | 14.87 | O |
| ATOM | 1513 | CB | MET | A | 214 | -1.441 | 1.901 | 27.899 | 1.00 | 14.50 | C |
| ATOM | 1514 | CG | MET | A | 214 | -0.707 | 0.864 | 28.744 | 1.00 | 14.52 | C |
| ATOM | 1515 | SD | MET | A | 214 | -1.317 | -0.822 | 28.524 | 1.00 | 14.52 | S |
| ATOM | 1516 | CE | MET | A | 214 | -0.293 | -1.699 | 29.695 | 1.00 | 14.80 | C |
| ATOM | 1517 | N | THR | A | 215 | -1.503 | 3.817 | 25.178 | 1.00 | 14.76 | N |
| ATOM | 1518 | CA | THR | A | 215 | -2.176 | 4.841 | 24.375 | 1.00 | 15.24 | C |
| ATOM | 1519 | C | THR | A | 215 | -2.098 | 4.542 | 22.878 | 1.00 | 15.36 | C |
| ATOM | 1520 | O | THR | A | 215 | -2.676 | 5.266 | 22.069 | 1.00 | 15.43 | O |
| ATOM | 1521 | CB | THR | A | 215 | -1.605 | 6.252 | 24.654 | 1.00 | 15.24 | C |
| ATOM | 1522 | OG1 | THR | A | 215 | -0.171 | 6.215 | 24.620 | 1.00 | 15.77 | O |
| ATOM | 1523 | CG2 | THR | A | 215 | -1.931 | 6.709 | 26.067 | 1.00 | 15.02 | C |
| ATOM | 1524 | N | PHE | A | 216 | -1.386 | 3.471 | 22.528 | 1.00 | 15.82 | N |
| ATOM | 1525 | CA | PHE | A | 216 | -1.163 | 3.047 | 21.138 | 1.00 | 16.27 | C |
| ATOM | 1526 | C | PHE | A | 216 | -0.301 | 4.028 | 20.340 | 1.00 | 16.46 | C |
| ATOM | 1527 | O | PHE | A | 216 | -0.621 | 4.372 | 19.197 | 1.00 | 16.56 | O |
| ATOM | 1528 | CB | PHE | A | 216 | -2.483 | 2.736 | 20.409 | 1.00 | 16.29 | C |
| ATOM | 1529 | CG | PHE | A | 216 | -3.254 | 1.588 | 21.004 | 1.00 | 16.75 | C |
| ATOM | 1530 | CD1 | PHE | A | 216 | -2.795 | 0.279 | 20.876 | 1.00 | 16.68 | C |
| ATOM | 1531 | CE1 | PHE | A | 216 | -3.508 | -0.786 | 21.429 | 1.00 | 16.75 | C |
| ATOM | 1532 | CZ | PHE | A | 216 | -4.692 | -0.546 | 22.117 | 1.00 | 16.83 | C |
| ATOM | 1533 | CE2 | PHE | A | 216 | -5.162 | 0.758 | 22.252 | 1.00 | 16.98 | C |
| ATOM | 1534 | CD2 | PHE | A | 216 | -4.441 | 1.818 | 21.696 | 1.00 | 16.92 | C |
| ATOM | 1535 | N | GLY | A | 217 | 0.788 | 4.474 | 20.961 | 1.00 | 16.52 | N |
| ATOM | 1536 | CA | GLY | A | 217 | 1.786 | 5.292 | 20.297 | 1.00 | 16.86 | C |
| ATOM | 1537 | C | GLY | A | 217 | 1.638 | 6.794 | 20.443 | 1.00 | 17.27 | C |
| ATOM | 1538 | O | GLY | A | 217 | 2.250 | 7.548 | 19.682 | 1.00 | 17.35 | O |
| ATOM | 1539 | N | SER | A | 218 | 0.840 | 7.234 | 21.412 | 1.00 | 17.71 | N |
| ATOM | 1540 | CA | SER | A | 218 | 0.640 | 8.664 | 21.644 | 1.00 | 18.33 | C |
| ATOM | 1541 | C | SER | A | 218 | 1.924 | 9.346 | 22.106 | 1.00 | 18.70 | C |
| ATOM | 1542 | O | SER | A | 218 | 2.709 | 8.775 | 22.868 | 1.00 | 18.74 | O |
| ATOM | 1543 | CB | SER | A | 218 | -0.480 | 8.913 | 22.656 | 1.00 | 18.30 | C |
| ATOM | 1544 | OG | SER | A | 218 | -1.756 | 8.825 | 22.041 | 1.00 | 18.54 | O |
| ATOM | 1545 | N | LYS | A | 219 | 2.131 | 10.566 | 21.622 | 1.00 | 19.16 | N |
| ATOM | 1546 | CA | LYS | A | 219 | 3.287 | 11.363 | 21.999 | 1.00 | 19.67 | C |
| ATOM | 1547 | C | LYS | A | 219 | 3.065 | 11.969 | 23.385 | 1.00 | 19.95 | C |
| ATOM | 1548 | O | LYS | A | 219 | 2.010 | 12.557 | 23.643 | 1.00 | 19.87 | O |
| ATOM | 1549 | CB | LYS | A | 219 | 3.540 | 12.455 | 20.959 | 1.00 | 19.75 | C |
| ATOM | 1550 | CG | LYS | A | 219 | 4.225 | 11.950 | 19.704 | 1.00 | 20.07 | C |
| ATOM | 1551 | CD | LYS | A | 219 | 4.205 | 12.991 | 18.598 | 1.00 | 21.12 | C |
| ATOM | 1552 | CE | LYS | A | 219 | 4.475 | 12.355 | 17.239 | 1.00 | 21.85 | C |
| ATOM | 1553 | NZ | LYS | A | 219 | 5.854 | 11.786 | 17.141 | 1.00 | 22.77 | N |
| ATOM | 1554 | N | PRO | A | 220 | 4.048 | 11.821 | 24.276 | 1.00 | 20.25 | N |
| ATOM | 1555 | CA | PRO | A | 220 | 3.914 | 12.303 | 25.659 | 1.00 | 20.59 | C |

FIG. 4Z

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1556 | C | PRO | A | 220 | 3.969 | 13.826 | 25.743 | 1.00 | 20.84 | C |
| ATOM | 1557 | O | PRO | A | 220 | 4.730 | 14.445 | 24.992 | 1.00 | 20.97 | O |
| ATOM | 1558 | CB | PRO | A | 220 | 5.115 | 11.671 | 26.373 | 1.00 | 20.53 | C |
| ATOM | 1559 | CG | PRO | A | 220 | 6.122 | 11.431 | 25.294 | 1.00 | 20.45 | C |
| ATOM | 1560 | CD | PRO | A | 220 | 5.358 | 11.190 | 24.028 | 1.00 | 19.99 | C |
| ATOM | 1561 | N | TYR | A | 221 | 3.164 | 14.401 | 26.638 | 1.00 | 21.13 | N |
| ATOM | 1562 | CA | TYR | A | 221 | 3.043 | 15.855 | 26.825 | 1.00 | 21.55 | C |
| ATOM | 1563 | C | TYR | A | 221 | 3.050 | 16.638 | 25.509 | 1.00 | 21.95 | C |
| ATOM | 1564 | O | TYR | A | 221 | 3.931 | 17.472 | 25.284 | 1.00 | 21.96 | O |
| ATOM | 1565 | CB | TYR | A | 221 | 4.147 | 16.398 | 27.740 | 1.00 | 21.40 | C |
| ATOM | 1566 | CG | TYR | A | 221 | 4.495 | 15.553 | 28.944 | 1.00 | 21.04 | C |
| ATOM | 1567 | CD1 | TYR | A | 221 | 3.767 | 15.655 | 30.128 | 1.00 | 20.62 | C |
| ATOM | 1568 | CE1 | TYR | A | 221 | 4.097 | 14.886 | 31.241 | 1.00 | 20.61 | C |
| ATOM | 1569 | CZ | TYR | A | 221 | 5.176 | 14.018 | 31.178 | 1.00 | 20.46 | C |
| ATOM | 1570 | OH | TYR | A | 221 | 5.512 | 13.258 | 32.272 | 1.00 | 20.34 | O |
| ATOM | 1571 | CE2 | TYR | A | 221 | 5.916 | 13.905 | 30.017 | 1.00 | 20.67 | C |
| ATOM | 1572 | CD2 | TYR | A | 221 | 5.578 | 14.677 | 28.909 | 1.00 | 20.98 | C |
| ATOM | 1573 | N | ASP | A | 222 | 2.068 | 16.372 | 24.652 | 1.00 | 22.48 | N |
| ATOM | 1574 | CA | ASP | A | 222 | 2.032 | 16.957 | 23.309 | 1.00 | 23.20 | C |
| ATOM | 1575 | C | ASP | A | 222 | 2.046 | 18.493 | 23.262 | 1.00 | 23.22 | C |
| ATOM | 1576 | O | ASP | A | 222 | 2.841 | 19.085 | 22.527 | 1.00 | 23.57 | O |
| ATOM | 1577 | CB | ASP | A | 222 | 0.847 | 16.413 | 22.506 | 1.00 | 23.36 | C |
| ATOM | 1578 | CG | ASP | A | 222 | 1.030 | 16.595 | 21.016 | 1.00 | 23.98 | C |
| ATOM | 1579 | OD1 | ASP | A | 222 | 0.866 | 17.734 | 20.528 | 1.00 | 24.37 | O |
| ATOM | 1580 | OD2 | ASP | A | 222 | 1.348 | 15.659 | 20.253 | 1.00 | 25.14 | O |
| ATOM | 1581 | N | GLY | A | 223 | 1.173 | 19.130 | 24.036 | 1.00 | 23.04 | N |
| ATOM | 1582 | CA | GLY | A | 223 | 1.078 | 20.581 | 24.038 | 1.00 | 23.08 | C |
| ATOM | 1583 | C | GLY | A | 223 | 2.113 | 21.293 | 24.894 | 1.00 | 22.99 | C |
| ATOM | 1584 | O | GLY | A | 223 | 2.182 | 22.525 | 24.894 | 1.00 | 22.94 | O |
| ATOM | 1585 | N | ILE | A | 224 | 2.915 | 20.518 | 25.621 | 1.00 | 22.70 | N |
| ATOM | 1586 | CA | ILE | A | 224 | 3.926 | 21.064 | 26.519 | 1.00 | 22.37 | C |
| ATOM | 1587 | C | ILE | A | 224 | 5.310 | 20.965 | 25.879 | 1.00 | 22.21 | C |
| ATOM | 1588 | O | ILE | A | 224 | 5.753 | 19.871 | 25.528 | 1.00 | 22.31 | O |
| ATOM | 1589 | CB | ILE | A | 224 | 3.913 | 20.328 | 27.896 | 1.00 | 22.38 | C |
| ATOM | 1590 | CG1 | ILE | A | 224 | 2.506 | 19.811 | 28.262 | 1.00 | 22.35 | C |
| ATOM | 1591 | CD1 | ILE | A | 224 | 1.467 | 20.885 | 28.597 | 1.00 | 22.43 | C |
| ATOM | 1592 | CG2 | ILE | A | 224 | 4.521 | 21.206 | 28.995 | 1.00 | 22.12 | C |
| ATOM | 1593 | N | PRO | A | 225 | 5.986 | 22.101 | 25.709 | 1.00 | 21.92 | N |
| ATOM | 1594 | CA | PRO | A | 225 | 7.373 | 22.096 | 25.227 | 1.00 | 21.76 | C |
| ATOM | 1595 | C | PRO | A | 225 | 8.339 | 21.573 | 26.293 | 1.00 | 21.65 | C |
| ATOM | 1596 | O | PRO | A | 225 | 8.026 | 21.623 | 27.484 | 1.00 | 21.75 | O |
| ATOM | 1597 | CB | PRO | A | 225 | 7.649 | 23.571 | 24.906 | 1.00 | 21.74 | C |
| ATOM | 1598 | CG | PRO | A | 225 | 6.652 | 24.350 | 25.681 | 1.00 | 21.88 | C |
| ATOM | 1599 | CD | PRO | A | 225 | 5.475 | 23.464 | 25.942 | 1.00 | 21.78 | C |
| ATOM | 1600 | N | ALA | A | 226 | 9.493 | 21.076 | 25.857 | 1.00 | 21.56 | N |
| ATOM | 1601 | CA | ALA | A | 226 | 10.479 | 20.464 | 26.750 | 1.00 | 21.30 | C |
| ATOM | 1602 | C | ALA | A | 226 | 10.953 | 21.395 | 27.867 | 1.00 | 21.14 | C |
| ATOM | 1603 | O | ALA | A | 226 | 11.230 | 20.943 | 28.983 | 1.00 | 21.18 | O |
| ATOM | 1604 | CB | ALA | A | 226 | 11.665 | 19.943 | 25.949 | 1.00 | 21.35 | C |
| ATOM | 1605 | N | SER | A | 227 | 11.031 | 22.690 | 27.564 | 1.00 | 20.82 | N |
| ATOM | 1606 | CA | SER | A | 227 | 11.462 | 23.698 | 28.532 | 1.00 | 20.42 | C |
| ATOM | 1607 | C | SER | A | 227 | 10.447 | 23.936 | 29.653 | 1.00 | 20.22 | C |
| ATOM | 1608 | O | SER | A | 227 | 10.774 | 24.552 | 30.667 | 1.00 | 20.39 | O |
| ATOM | 1609 | CB | SER | A | 227 | 11.810 | 25.017 | 27.825 | 1.00 | 20.47 | C |
| ATOM | 1610 | OG | SER | A | 227 | 10.706 | 25.543 | 27.106 | 1.00 | 20.20 | O |
| ATOM | 1611 | N | GLU | A | 228 | 9.228 | 23.432 | 29.472 | 1.00 | 20.06 | N |
| ATOM | 1612 | CA | GLU | A | 228 | 8.161 | 23.573 | 30.467 | 1.00 | 19.96 | C |
| ATOM | 1613 | C | GLU | A | 228 | 7.863 | 22.284 | 31.249 | 1.00 | 19.60 | C |
| ATOM | 1614 | O | GLU | A | 228 | 7.043 | 22.291 | 32.170 | 1.00 | 19.60 | O |
| ATOM | 1615 | CB | GLU | A | 228 | 6.876 | 24.084 | 29.803 | 1.00 | 20.13 | C |

FIG. 4AA

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1616 | CG | GLU | A | 228 | 7.016 | 25.425 | 29.098 | 1.00 | 20.70 | C |
| ATOM | 1617 | CD | GLU | A | 228 | 7.139 | 26.594 | 30.057 | 1.00 | 21.48 | C |
| ATOM | 1618 | OE1 | GLU | A | 228 | 6.474 | 26.579 | 31.114 | 1.00 | 21.87 | O |
| ATOM | 1619 | OE2 | GLU | A | 228 | 7.903 | 27.534 | 29.748 | 1.00 | 22.07 | O |
| ATOM | 1620 | N | ILE | A | 229 | 8.536 | 21.193 | 30.885 | 1.00 | 19.27 | N |
| ATOM | 1621 | CA | ILE | A | 229 | 8.304 | 19.875 | 31.486 | 1.00 | 19.00 | C |
| ATOM | 1622 | C | ILE | A | 229 | 8.592 | 19.813 | 32.997 | 1.00 | 18.87 | C |
| ATOM | 1623 | O | ILE | A | 229 | 7.751 | 19.344 | 33.767 | 1.00 | 18.73 | O |
| ATOM | 1624 | CB | ILE | A | 229 | 9.094 | 18.772 | 30.711 | 1.00 | 18.98 | C |
| ATOM | 1625 | CG1 | ILE | A | 229 | 8.512 | 18.560 | 29.303 | 1.00 | 18.73 | C |
| ATOM | 1626 | CD1 | ILE | A | 229 | 7.059 | 18.094 | 29.254 | 1.00 | 17.92 | C |
| ATOM | 1627 | CG2 | ILE | A | 229 | 9.154 | 17.462 | 31.502 | 1.00 | 18.78 | C |
| ATOM | 1628 | N | SER | A | 230 | 9.764 | 20.291 | 33.414 | 1.00 | 18.76 | N |
| ATOM | 1629 | CA | SER | A | 230 | 10.130 | 20.307 | 34.836 | 1.00 | 18.71 | C |
| ATOM | 1630 | C | SER | A | 230 | 9.120 | 21.081 | 35.681 | 1.00 | 18.57 | C |
| ATOM | 1631 | O | SER | A | 230 | 8.848 | 20.706 | 36.821 | 1.00 | 18.28 | O |
| ATOM | 1632 | CB | SER | A | 230 | 11.543 | 20.862 | 35.045 | 1.00 | 18.69 | C |
| ATOM | 1633 | OG | SER | A | 230 | 11.636 | 22.209 | 34.616 | 1.00 | 19.01 | O |
| ATOM | 1634 | N | SER | A | 231 | 8.560 | 22.145 | 35.106 | 1.00 | 18.63 | N |
| ATOM | 1635 | CA | SER | A | 231 | 7.543 | 22.957 | 35.774 | 1.00 | 18.67 | C |
| ATOM | 1636 | C | SER | A | 231 | 6.243 | 22.190 | 36.022 | 1.00 | 18.74 | C |
| ATOM | 1637 | O | SER | A | 231 | 5.755 | 22.151 | 37.152 | 1.00 | 19.01 | O |
| ATOM | 1638 | CB | SER | A | 231 | 7.262 | 24.241 | 34.987 | 1.00 | 18.56 | C |
| ATOM | 1639 | OG | SER | A | 231 | 6.154 | 24.935 | 35.537 | 1.00 | 18.36 | O |
| ATOM | 1640 | N | ILE | A | 232 | 5.689 | 21.577 | 34.977 | 1.00 | 18.72 | N |
| ATOM | 1641 | CA | ILE | A | 232 | 4.453 | 20.805 | 35.129 | 1.00 | 18.83 | C |
| ATOM | 1642 | C | ILE | A | 232 | 4.616 | 19.598 | 36.072 | 1.00 | 18.81 | C |
| ATOM | 1643 | O | ILE | A | 232 | 3.690 | 19.259 | 36.805 | 1.00 | 18.86 | O |
| ATOM | 1644 | CB | ILE | A | 232 | 3.820 | 20.398 | 33.747 | 1.00 | 18.91 | C |
| ATOM | 1645 | CG1 | ILE | A | 232 | 4.626 | 19.301 | 33.041 | 1.00 | 18.56 | C |
| ATOM | 1646 | CD1 | ILE | A | 232 | 3.938 | 17.960 | 33.036 | 1.00 | 17.74 | C |
| ATOM | 1647 | CG2 | ILE | A | 232 | 3.645 | 21.613 | 32.835 | 1.00 | 18.82 | C |
| ATOM | 1648 | N | LEU | A | 233 | 5.797 | 18.978 | 36.067 | 1.00 | 18.80 | N |
| ATOM | 1649 | CA | LEU | A | 233 | 6.066 | 17.816 | 36.920 | 1.00 | 18.77 | C |
| ATOM | 1650 | C | LEU | A | 233 | 6.152 | 18.182 | 38.402 | 1.00 | 18.86 | C |
| ATOM | 1651 | O | LEU | A | 233 | 5.641 | 17.452 | 39.253 | 1.00 | 18.77 | O |
| ATOM | 1652 | CB | LEU | A | 233 | 7.342 | 17.087 | 36.480 | 1.00 | 18.68 | C |
| ATOM | 1653 | CG | LEU | A | 233 | 7.376 | 16.345 | 35.140 | 1.00 | 18.50 | C |
| ATOM | 1654 | CD1 | LEU | A | 233 | 8.783 | 15.844 | 34.869 | 1.00 | 18.03 | C |
| ATOM | 1655 | CD2 | LEU | A | 233 | 6.374 | 15.193 | 35.077 | 1.00 | 18.39 | C |
| ATOM | 1656 | N | GLU | A | 234 | 6.792 | 19.314 | 38.700 | 1.00 | 19.10 | N |
| ATOM | 1657 | CA | GLU | A | 234 | 6.897 | 19.812 | 40.077 | 1.00 | 19.27 | C |
| ATOM | 1658 | C | GLU | A | 234 | 5.551 | 20.344 | 40.582 | 1.00 | 19.12 | C |
| ATOM | 1659 | O | GLU | A | 234 | 5.321 | 20.430 | 41.791 | 1.00 | 18.98 | O |
| ATOM | 1660 | CB | GLU | A | 234 | 7.990 | 20.888 | 40.207 | 1.00 | 19.22 | C |
| ATOM | 1661 | CG | GLU | A | 234 | 9.411 | 20.394 | 39.944 | 1.00 | 19.78 | C |
| ATOM | 1662 | CD | GLU | A | 234 | 10.129 | 19.880 | 41.185 | 1.00 | 20.57 | C |
| ATOM | 1663 | OE1 | GLU | A | 234 | 11.362 | 20.076 | 41.279 | 1.00 | 20.95 | O |
| ATOM | 1664 | OE2 | GLU | A | 234 | 9.479 | 19.267 | 42.060 | 1.00 | 20.64 | O |
| ATOM | 1665 | N | LYS | A | 235 | 4.668 | 20.687 | 39.646 | 1.00 | 19.06 | N |
| ATOM | 1666 | CA | LYS | A | 235 | 3.316 | 21.136 | 39.966 | 1.00 | 18.94 | C |
| ATOM | 1667 | C | LYS | A | 235 | 2.381 | 19.963 | 40.271 | 1.00 | 18.93 | C |
| ATOM | 1668 | O | LYS | A | 235 | 1.229 | 20.164 | 40.668 | 1.00 | 18.95 | O |
| ATOM | 1669 | CB | LYS | A | 235 | 2.755 | 21.984 | 38.823 | 1.00 | 18.92 | C |
| ATOM | 1670 | CG | LYS | A | 235 | 2.836 | 23.482 | 39.069 | 1.00 | 18.70 | C |
| ATOM | 1671 | CD | LYS | A | 235 | 3.254 | 24.227 | 37.818 | 1.00 | 18.66 | C |
| ATOM | 1672 | CE | LYS | A | 235 | 2.903 | 25.703 | 37.907 | 1.00 | 19.05 | C |
| ATOM | 1673 | NZ | LYS | A | 235 | 1.961 | 26.119 | 36.830 | 1.00 | 19.31 | N |
| ATOM | 1674 | N | GLY | A | 236 | 2.885 | 18.744 | 40.090 | 1.00 | 18.81 | N |
| ATOM | 1675 | CA | GLY | A | 236 | 2.120 | 17.537 | 40.348 | 1.00 | 18.41 | C |

FIG. 4BB

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1676 | C | GLY | A | 236 | 1.517 | 16.921 | 39.100 | 1.00 | 18.28 | C |
| ATOM | 1677 | O | GLY | A | 236 | 0.925 | 15.846 | 39.164 | 1.00 | 18.52 | O |
| ATOM | 1678 | N | GLU | A | 237 | 1.668 | 17.599 | 37.965 | 1.00 | 18.11 | N |
| ATOM | 1679 | CA | GLU | A | 237 | 1.069 | 17.151 | 36.713 | 1.00 | 17.92 | C |
| ATOM | 1680 | C | GLU | A | 237 | 1.799 | 15.953 | 36.116 | 1.00 | 17.69 | C |
| ATOM | 1681 | O | GLU | A | 237 | 3.032 | 15.945 | 36.001 | 1.00 | 17.32 | O |
| ATOM | 1682 | CB | GLU | A | 237 | 1.020 | 18.287 | 35.698 | 1.00 | 18.19 | C |
| ATOM | 1683 | CG | GLU | A | 237 | -0.243 | 19.122 | 35.762 | 1.00 | 18.82 | C |
| ATOM | 1684 | CD | GLU | A | 237 | -0.084 | 20.450 | 35.057 | 1.00 | 19.23 | C |
| ATOM | 1685 | OE1 | GLU | A | 237 | -0.016 | 20.455 | 33.808 | 1.00 | 19.67 | O |
| ATOM | 1686 | OE2 | GLU | A | 237 | -0.020 | 21.483 | 35.754 | 1.00 | 19.42 | O |
| ATOM | 1687 | N | ARG | A | 238 | 1.014 | 14.947 | 35.739 | 1.00 | 17.15 | N |
| ATOM | 1688 | CA | ARG | A | 238 | 1.535 | 13.720 | 35.157 | 1.00 | 16.62 | C |
| ATOM | 1689 | C | ARG | A | 238 | 0.815 | 13.418 | 33.848 | 1.00 | 16.48 | C |
| ATOM | 1690 | O | ARG | A | 238 | -0.066 | 14.171 | 33.431 | 1.00 | 16.46 | O |
| ATOM | 1691 | CB | ARG | A | 238 | 1.384 | 12.559 | 36.147 | 1.00 | 16.54 | C |
| ATOM | 1692 | CG | ARG | A | 238 | 2.203 | 12.700 | 37.431 | 1.00 | 16.13 | C |
| ATOM | 1693 | CD | ARG | A | 238 | 3.705 | 12.514 | 37.243 | 1.00 | 15.74 | C |
| ATOM | 1694 | NE | ARG | A | 238 | 4.444 | 12.574 | 38.504 | 1.00 | 15.07 | N |
| ATOM | 1695 | CZ | ARG | A | 238 | 4.911 | 13.692 | 39.055 | 1.00 | 14.75 | C |
| ATOM | 1696 | NH1 | ARG | A | 238 | 4.720 | 14.868 | 38.470 | 1.00 | 14.70 | N |
| ATOM | 1697 | NH2 | ARG | A | 238 | 5.572 | 13.636 | 40.200 | 1.00 | 14.39 | N |
| ATOM | 1698 | N | LEU | A | 239 | 1.201 | 12.323 | 33.196 | 1.00 | 16.31 | N |
| ATOM | 1699 | CA | LEU | A | 239 | 0.558 | 11.895 | 31.957 | 1.00 | 16.06 | C |
| ATOM | 1700 | C | LEU | A | 239 | -0.842 | 11.341 | 32.235 | 1.00 | 15.95 | C |
| ATOM | 1701 | O | LEU | A | 239 | -1.054 | 10.670 | 33.245 | 1.00 | 15.97 | O |
| ATOM | 1702 | CB | LEU | A | 239 | 1.427 | 10.862 | 31.226 | 1.00 | 16.07 | C |
| ATOM | 1703 | CG | LEU | A | 239 | 2.710 | 11.394 | 30.570 | 1.00 | 15.69 | C |
| ATOM | 1704 | CD1 | LEU | A | 239 | 3.752 | 10.297 | 30.453 | 1.00 | 15.56 | C |
| ATOM | 1705 | CD2 | LEU | A | 239 | 2.437 | 12.016 | 29.207 | 1.00 | 15.32 | C |
| ATOM | 1706 | N | PRO | A | 240 | -1.797 | 11.632 | 31.350 | 1.00 | 15.91 | N |
| ATOM | 1707 | CA | PRO | A | 240 | -3.195 | 11.232 | 31.563 | 1.00 | 15.92 | C |
| ATOM | 1708 | C | PRO | A | 240 | -3.401 | 9.716 | 31.537 | 1.00 | 16.15 | C |
| ATOM | 1709 | O | PRO | A | 240 | -2.642 | 8.998 | 30.882 | 1.00 | 16.12 | O |
| ATOM | 1710 | CB | PRO | A | 240 | -3.928 | 11.889 | 30.390 | 1.00 | 15.96 | C |
| ATOM | 1711 | CG | PRO | A | 240 | -2.887 | 12.080 | 29.343 | 1.00 | 15.71 | C |
| ATOM | 1712 | CD | PRO | A | 240 | -1.619 | 12.363 | 30.081 | 1.00 | 15.78 | C |
| ATOM | 1713 | N | GLN | A | 241 | -4.423 | 9.249 | 32.251 | 1.00 | 16.28 | N |
| ATOM | 1714 | CA | GLN | A | 241 | -4.776 | 7.834 | 32.289 | 1.00 | 16.22 | C |
| ATOM | 1715 | C | GLN | A | 241 | -5.318 | 7.370 | 30.937 | 1.00 | 16.41 | C |
| ATOM | 1716 | O | GLN | A | 241 | -6.339 | 7.880 | 30.476 | 1.00 | 16.31 | O |
| ATOM | 1717 | CB | GLN | A | 241 | -5.807 | 7.580 | 33.392 | 1.00 | 16.16 | C |
| ATOM | 1718 | CG | GLN | A | 241 | -6.396 | 6.169 | 33.416 | 1.00 | 15.84 | C |
| ATOM | 1719 | CD | GLN | A | 241 | -7.098 | 5.847 | 34.722 | 1.00 | 16.00 | C |
| ATOM | 1720 | OE1 | GLN | A | 241 | -7.395 | 6.746 | 35.513 | 1.00 | 15.65 | O |
| ATOM | 1721 | NE2 | GLN | A | 241 | -7.365 | 4.563 | 34.953 | 1.00 | 15.90 | N |
| ATOM | 1722 | N | PRO | A | 242 | -4.641 | 6.408 | 30.305 | 1.00 | 16.79 | N |
| ATOM | 1723 | CA | PRO | A | 242 | -5.093 | 5.872 | 29.015 | 1.00 | 17.07 | C |
| ATOM | 1724 | C | PRO | A | 242 | -6.456 | 5.189 | 29.143 | 1.00 | 17.34 | C |
| ATOM | 1725 | O | PRO | A | 242 | -6.669 | 4.466 | 30.120 | 1.00 | 17.35 | O |
| ATOM | 1726 | CB | PRO | A | 242 | -4.005 | 4.855 | 28.655 | 1.00 | 16.94 | C |
| ATOM | 1727 | CG | PRO | A | 242 | -2.824 | 5.262 | 29.467 | 1.00 | 16.93 | C |
| ATOM | 1728 | CD | PRO | A | 242 | -3.397 | 5.759 | 30.759 | 1.00 | 16.83 | C |
| ATOM | 1729 | N | PRO | A | 243 | -7.358 | 5.437 | 28.188 | 1.00 | 17.55 | N |
| ATOM | 1730 | CA | PRO | A | 243 | -8.723 | 4.884 | 28.207 | 1.00 | 17.67 | C |
| ATOM | 1731 | C | PRO | A | 243 | -8.818 | 3.395 | 28.553 | 1.00 | 17.80 | C |
| ATOM | 1732 | O | PRO | A | 243 | -9.696 | 3.017 | 29.325 | 1.00 | 18.11 | O |
| ATOM | 1733 | CB | PRO | A | 243 | -9.210 | 5.119 | 26.774 | 1.00 | 17.61 | C |
| ATOM | 1734 | CG | PRO | A | 243 | -8.473 | 6.326 | 26.321 | 1.00 | 17.59 | C |
| ATOM | 1735 | CD | PRO | A | 243 | -7.136 | 6.304 | 27.015 | 1.00 | 17.41 | C |

FIG. 4CC

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1736 | N | ILE | A | 244 | -7.929 | 2.575 | 28.003 | 1.00 | 18.01 | N |
| ATOM | 1737 | CA | ILE | A | 244 | -7.974 | 1.125 | 28.211 | 1.00 | 18.27 | C |
| ATOM | 1738 | C | ILE | A | 244 | -7.446 | 0.673 | 29.580 | 1.00 | 18.61 | C |
| ATOM | 1739 | O | ILE | A | 244 | -7.552 | -0.509 | 29.928 | 1.00 | 18.60 | O |
| ATOM | 1740 | CB | ILE | A | 244 | -7.228 | 0.372 | 27.066 | 1.00 | 18.29 | C |
| ATOM | 1741 | CG1 | ILE | A | 244 | -5.718 | 0.636 | 27.127 | 1.00 | 18.33 | C |
| ATOM | 1742 | CD1 | ILE | A | 244 | -4.873 | -0.598 | 26.924 | 1.00 | 18.55 | C |
| ATOM | 1743 | CG2 | ILE | A | 244 | -7.808 | 0.739 | 25.697 | 1.00 | 17.76 | C |
| ATOM | 1744 | N | CYS | A | 245 | -6.894 | 1.611 | 30.350 | 1.00 | 18.75 | N |
| ATOM | 1745 | CA | CYS | A | 245 | -6.241 | 1.294 | 31.621 | 1.00 | 18.94 | C |
| ATOM | 1746 | C | CYS | A | 245 | -7.163 | 1.371 | 32.835 | 1.00 | 19.33 | C |
| ATOM | 1747 | O | CYS | A | 245 | -7.803 | 2.401 | 33.076 | 1.00 | 19.54 | O |
| ATOM | 1748 | CB | CYS | A | 245 | -5.045 | 2.219 | 31.850 | 1.00 | 18.88 | C |
| ATOM | 1749 | SG | CYS | A | 245 | -3.640 | 1.920 | 30.767 | 1.00 | 18.26 | S |
| ATOM | 1750 | N | THR | A | 246 | -7.209 | 0.282 | 33.601 | 1.00 | 19.58 | N |
| ATOM | 1751 | CA | THR | A | 246 | -7.842 | 0.285 | 34.919 | 1.00 | 19.83 | C |
| ATOM | 1752 | C | THR | A | 246 | -6.909 | 0.989 | 35.901 | 1.00 | 20.24 | C |
| ATOM | 1753 | O | THR | A | 246 | -5.705 | 1.103 | 35.645 | 1.00 | 20.07 | O |
| ATOM | 1754 | CB | THR | A | 246 | -8.133 | -1.149 | 35.412 | 1.00 | 19.83 | C |
| ATOM | 1755 | OG1 | THR | A | 246 | -6.934 | -1.932 | 35.349 | 1.00 | 19.85 | O |
| ATOM | 1756 | CG2 | THR | A | 246 | -9.100 | -1.875 | 34.475 | 1.00 | 19.57 | C |
| ATOM | 1757 | N | ILE | A | 247 | -7.462 | 1.442 | 37.026 | 1.00 | 20.58 | N |
| ATOM | 1758 | CA | ILE | A | 247 | -6.696 | 2.196 | 38.018 | 1.00 | 21.02 | C |
| ATOM | 1759 | C | ILE | A | 247 | -5.422 | 1.480 | 38.486 | 1.00 | 21.30 | C |
| ATOM | 1760 | O | ILE | A | 247 | -4.440 | 2.132 | 38.836 | 1.00 | 21.66 | O |
| ATOM | 1761 | CB | ILE | A | 247 | -7.601 | 2.625 | 39.217 | 1.00 | 21.12 | C |
| ATOM | 1762 | CG1 | ILE | A | 247 | -7.055 | 3.896 | 39.879 | 1.00 | 21.08 | C |
| ATOM | 1763 | CG2 | ILE | A | 247 | -7.773 | 1.492 | 40.237 | 1.00 | 21.11 | C |
| ATOM | 1764 | N | ASP | A | 248 | -5.445 | 0.148 | 38.468 | 1.00 | 21.38 | N |
| ATOM | 1765 | CA | ASP | A | 248 | -4.304 | -0.669 | 38.876 | 1.00 | 21.33 | C |
| ATOM | 1766 | C | ASP | A | 248 | -3.125 | -0.552 | 37.911 | 1.00 | 21.12 | C |
| ATOM | 1767 | O | ASP | A | 248 | -1.973 | -0.521 | 38.342 | 1.00 | 21.35 | O |
| ATOM | 1768 | CB | ASP | A | 248 | -4.721 | -2.137 | 39.016 | 1.00 | 21.74 | C |
| ATOM | 1769 | CG | ASP | A | 248 | -4.978 | -2.543 | 40.458 | 1.00 | 22.18 | C |
| ATOM | 1770 | OD1 | ASP | A | 248 | -5.164 | -3.753 | 40.710 | 1.00 | 22.94 | O |
| ATOM | 1771 | OD2 | ASP | A | 248 | -5.013 | -1.730 | 41.406 | 1.00 | 22.65 | O |
| ATOM | 1772 | N | VAL | A | 249 | -3.415 | -0.498 | 36.612 | 1.00 | 20.65 | N |
| ATOM | 1773 | CA | VAL | A | 249 | -2.374 | -0.357 | 35.594 | 1.00 | 20.23 | C |
| ATOM | 1774 | C | VAL | A | 249 | -1.845 | 1.078 | 35.553 | 1.00 | 19.95 | C |
| ATOM | 1775 | O | VAL | A | 249 | -0.646 | 1.296 | 35.370 | 1.00 | 20.00 | O |
| ATOM | 1776 | CB | VAL | A | 249 | -2.860 | -0.798 | 34.185 | 1.00 | 20.14 | C |
| ATOM | 1777 | CG1 | VAL | A | 249 | -1.767 | -0.592 | 33.136 | 1.00 | 20.21 | C |
| ATOM | 1778 | CG2 | VAL | A | 249 | -3.293 | -2.250 | 34.197 | 1.00 | 19.95 | C |
| ATOM | 1779 | N | TYR | A | 250 | -2.740 | 2.046 | 35.731 | 1.00 | 19.73 | N |
| ATOM | 1780 | CA | TYR | A | 250 | -2.360 | 3.459 | 35.734 | 1.00 | 19.51 | C |
| ATOM | 1781 | C | TYR | A | 250 | -1.520 | 3.830 | 36.954 | 1.00 | 19.47 | C |
| ATOM | 1782 | O | TYR | A | 250 | -0.626 | 4.664 | 36.855 | 1.00 | 19.63 | O |
| ATOM | 1783 | CB | TYR | A | 250 | -3.591 | 4.368 | 35.632 | 1.00 | 19.26 | C |
| ATOM | 1784 | CG | TYR | A | 250 | -3.264 | 5.851 | 35.610 | 1.00 | 18.79 | C |
| ATOM | 1785 | CD1 | TYR | A | 250 | -3.859 | 6.728 | 36.517 | 1.00 | 17.98 | C |
| ATOM | 1786 | CE1 | TYR | A | 250 | -3.565 | 8.087 | 36.502 | 1.00 | 17.77 | C |
| ATOM | 1787 | CZ | TYR | A | 250 | -2.665 | 8.585 | 35.572 | 1.00 | 17.96 | C |
| ATOM | 1788 | OH | TYR | A | 250 | -2.374 | 9.927 | 35.557 | 1.00 | 17.47 | O |
| ATOM | 1789 | CE2 | TYR | A | 250 | -2.056 | 7.737 | 34.660 | 1.00 | 18.16 | C |
| ATOM | 1790 | CD2 | TYR | A | 250 | -2.359 | 6.377 | 34.681 | 1.00 | 18.36 | C |
| ATOM | 1791 | N | MET | A | 251 | -1.802 | 3.196 | 38.090 | 1.00 | 19.53 | N |
| ATOM | 1792 | CA | MET | A | 251 | -1.063 | 3.440 | 39.329 | 1.00 | 19.50 | C |
| ATOM | 1793 | C | MET | A | 251 | 0.399 | 3.008 | 39.262 | 1.00 | 19.37 | C |
| ATOM | 1794 | O | MET | A | 251 | 1.243 | 3.580 | 39.954 | 1.00 | 19.54 | O |
| ATOM | 1795 | CB | MET | A | 251 | -1.748 | 2.754 | 40.511 | 1.00 | 19.55 | C |

FIG. 4DD

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1796 | CG | MET | A | 251 | -2.869 | 3.569 | 41.127 | 1.00 | 19.98 | C |
| ATOM | 1797 | SD | MET | A | 251 | -2.379 | 5.234 | 41.621 | 1.00 | 20.75 | S |
| ATOM | 1798 | CE | MET | A | 251 | -1.468 | 4.872 | 43.146 | 1.00 | 20.68 | C |
| ATOM | 1799 | N | ILE | A | 252 | 0.689 | 2.002 | 38.438 | 1.00 | 19.21 | N |
| ATOM | 1800 | CA | ILE | A | 252 | 2.055 | 1.515 | 38.253 | 1.00 | 19.06 | C |
| ATOM | 1801 | C | ILE | A | 252 | 2.938 | 2.592 | 37.623 | 1.00 | 19.04 | C |
| ATOM | 1802 | O | ILE | A | 252 | 4.014 | 2.889 | 38.142 | 1.00 | 18.95 | O |
| ATOM | 1803 | CB | ILE | A | 252 | 2.075 | 0.202 | 37.418 | 1.00 | 19.10 | C |
| ATOM | 1804 | CG1 | ILE | A | 252 | 1.766 | -1.004 | 38.312 | 1.00 | 18.99 | C |
| ATOM | 1805 | CD1 | ILE | A | 252 | 1.608 | -2.317 | 37.560 | 1.00 | 19.04 | C |
| ATOM | 1806 | CG2 | ILE | A | 252 | 3.422 | 0.016 | 36.714 | 1.00 | 18.99 | C |
| ATOM | 1807 | N | MET | A | 253 | 2.477 | 3.181 | 36.519 | 1.00 | 19.01 | N |
| ATOM | 1808 | CA | MET | A | 253 | 3.243 | 4.228 | 35.838 | 1.00 | 19.12 | C |
| ATOM | 1809 | C | MET | A | 253 | 3.331 | 5.486 | 36.695 | 1.00 | 18.66 | C |
| ATOM | 1810 | O | MET | A | 253 | 4.376 | 6.135 | 36.734 | 1.00 | 18.54 | O |
| ATOM | 1811 | CB | MET | A | 253 | 2.692 | 4.550 | 34.435 | 1.00 | 19.34 | C |
| ATOM | 1812 | CG | MET | A | 253 | 1.258 | 4.113 | 34.173 | 1.00 | 20.34 | C |
| ATOM | 1813 | SD | MET | A | 253 | 0.800 | 4.219 | 32.431 | 1.00 | 21.21 | S |
| ATOM | 1814 | CE | MET | A | 253 | -0.398 | 2.920 | 32.333 | 1.00 | 21.00 | C |
| ATOM | 1815 | N | VAL | A | 254 | 2.237 | 5.807 | 37.388 | 1.00 | 18.26 | N |
| ATOM | 1816 | CA | VAL | A | 254 | 2.202 | 6.913 | 38.348 | 1.00 | 17.77 | C |
| ATOM | 1817 | C | VAL | A | 254 | 3.262 | 6.732 | 39.443 | 1.00 | 17.57 | C |
| ATOM | 1818 | O | VAL | A | 254 | 3.895 | 7.702 | 39.872 | 1.00 | 17.53 | O |
| ATOM | 1819 | CB | VAL | A | 254 | 0.785 | 7.094 | 38.960 | 1.00 | 17.70 | C |
| ATOM | 1820 | CG1 | VAL | A | 254 | 0.817 | 7.966 | 40.221 | 1.00 | 17.51 | C |
| ATOM | 1821 | CG2 | VAL | A | 254 | -0.156 | 7.698 | 37.936 | 1.00 | 17.34 | C |
| ATOM | 1822 | N | LYS | A | 255 | 3.460 | 5.486 | 39.870 | 1.00 | 17.14 | N |
| ATOM | 1823 | CA | LYS | A | 255 | 4.492 | 5.147 | 40.846 | 1.00 | 16.92 | C |
| ATOM | 1824 | C | LYS | A | 255 | 5.906 | 5.322 | 40.278 | 1.00 | 16.85 | C |
| ATOM | 1825 | O | LYS | A | 255 | 6.825 | 5.713 | 40.999 | 1.00 | 16.73 | O |
| ATOM | 1826 | CB | LYS | A | 255 | 4.293 | 3.720 | 41.361 | 1.00 | 16.79 | C |
| ATOM | 1827 | CG | LYS | A | 255 | 3.657 | 3.641 | 42.738 | 1.00 | 16.86 | C |
| ATOM | 1828 | N | CYS | A | 256 | 6.070 | 5.033 | 38.986 | 1.00 | 16.84 | N |
| ATOM | 1829 | CA | CYS | A | 256 | 7.348 | 5.210 | 38.295 | 1.00 | 16.76 | C |
| ATOM | 1830 | C | CYS | A | 256 | 7.744 | 6.689 | 38.186 | 1.00 | 17.05 | C |
| ATOM | 1831 | O | CYS | A | 256 | 8.917 | 7.006 | 37.978 | 1.00 | 17.06 | O |
| ATOM | 1832 | CB | CYS | A | 256 | 7.308 | 4.577 | 36.897 | 1.00 | 16.68 | C |
| ATOM | 1833 | SG | CYS | A | 256 | 6.894 | 2.809 | 36.822 | 1.00 | 16.67 | S |
| ATOM | 1834 | N | TRP | A | 257 | 6.766 | 7.584 | 38.336 | 1.00 | 17.20 | N |
| ATOM | 1835 | CA | TRP | A | 257 | 6.990 | 9.021 | 38.175 | 1.00 | 17.29 | C |
| ATOM | 1836 | C | TRP | A | 257 | 7.052 | 9.803 | 39.496 | 1.00 | 17.59 | C |
| ATOM | 1837 | O | TRP | A | 257 | 6.770 | 11.006 | 39.525 | 1.00 | 17.52 | O |
| ATOM | 1838 | CB | TRP | A | 257 | 5.932 | 9.632 | 37.249 | 1.00 | 17.24 | C |
| ATOM | 1839 | CG | TRP | A | 257 | 5.797 | 8.962 | 35.906 | 1.00 | 17.23 | C |
| ATOM | 1840 | CD1 | TRP | A | 257 | 6.798 | 8.421 | 35.148 | 1.00 | 16.77 | C |
| ATOM | 1841 | NE1 | TRP | A | 257 | 6.283 | 7.904 | 33.984 | 1.00 | 16.80 | N |
| ATOM | 1842 | CE2 | TRP | A | 257 | 4.928 | 8.104 | 33.966 | 1.00 | 16.76 | C |
| ATOM | 1843 | CD2 | TRP | A | 257 | 4.587 | 8.774 | 35.161 | 1.00 | 17.00 | C |
| ATOM | 1844 | CE3 | TRP | A | 257 | 3.240 | 9.098 | 35.387 | 1.00 | 17.15 | C |
| ATOM | 1845 | CZ3 | TRP | A | 257 | 2.295 | 8.752 | 34.424 | 1.00 | 17.26 | C |
| ATOM | 1846 | CH2 | TRP | A | 257 | 2.673 | 8.087 | 33.246 | 1.00 | 17.22 | C |
| ATOM | 1847 | CZ2 | TRP | A | 257 | 3.979 | 7.756 | 33.000 | 1.00 | 16.76 | C |
| ATOM | 1848 | N | MET | A | 258 | 7.430 | 9.125 | 40.578 | 1.00 | 17.84 | N |
| ATOM | 1849 | CA | MET | A | 258 | 7.608 | 9.779 | 41.875 | 1.00 | 18.16 | C |
| ATOM | 1850 | C | MET | A | 258 | 8.911 | 10.575 | 41.903 | 1.00 | 18.02 | C |
| ATOM | 1851 | O | MET | A | 258 | 9.950 | 10.085 | 41.457 | 1.00 | 17.98 | O |
| ATOM | 1852 | CB | MET | A | 258 | 7.612 | 8.751 | 43.013 | 1.00 | 18.55 | C |
| ATOM | 1853 | CG | MET | A | 258 | 6.344 | 7.913 | 43.129 | 1.00 | 19.22 | C |
| ATOM | 1854 | SD | MET | A | 258 | 5.036 | 8.729 | 44.044 | 1.00 | 20.53 | S |
| ATOM | 1855 | CE | MET | A | 258 | 3.632 | 7.680 | 43.650 | 1.00 | 20.24 | C |

FIG. 4EE

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1856 | N | ILE | A | 259 | 8.846 | 11.798 | 42.431 | 1.00 | 17.95 | N |
| ATOM | 1857 | CA | ILE | A | 259 | 10.022 | 12.661 | 42.582 | 1.00 | 17.79 | C |
| ATOM | 1858 | C | ILE | A | 259 | 11.094 | 11.995 | 43.455 | 1.00 | 17.91 | C |
| ATOM | 1859 | O | ILE | A | 259 | 12.285 | 12.090 | 43.161 | 1.00 | 18.16 | O |
| ATOM | 1860 | CB | ILE | A | 259 | 9.624 | 14.065 | 43.138 | 1.00 | 17.79 | C |
| ATOM | 1861 | CG1 | ILE | A | 259 | 8.462 | 14.678 | 42.337 | 1.00 | 17.48 | C |
| ATOM | 1862 | CD1 | ILE | A | 259 | 8.711 | 14.852 | 40.839 | 1.00 | 16.82 | C |
| ATOM | 1863 | CG2 | ILE | A | 259 | 10.836 | 15.017 | 43.191 | 1.00 | 17.37 | C |
| ATOM | 1864 | N | ASP | A | 260 | 10.664 | 11.317 | 44.517 | 1.00 | 18.02 | N |
| ATOM | 1865 | CA | ASP | A | 260 | 11.561 | 10.477 | 45.304 | 1.00 | 18.12 | C |
| ATOM | 1866 | C | ASP | A | 260 | 11.792 | 9.145 | 44.586 | 1.00 | 18.28 | C |
| ATOM | 1867 | O | ASP | A | 260 | 10.884 | 8.311 | 44.479 | 1.00 | 18.14 | O |
| ATOM | 1868 | CB | ASP | A | 260 | 11.012 | 10.251 | 46.715 | 1.00 | 18.08 | C |
| ATOM | 1869 | CG | ASP | A | 260 | 11.809 | 9.215 | 47.492 | 1.00 | 18.62 | C |
| ATOM | 1870 | OD1 | ASP | A | 260 | 11.221 | 8.184 | 47.877 | 1.00 | 19.78 | O |
| ATOM | 1871 | OD2 | ASP | A | 260 | 13.026 | 9.333 | 47.757 | 1.00 | 18.48 | O |
| ATOM | 1872 | N | ALA | A | 261 | 13.018 | 8.961 | 44.103 | 1.00 | 18.38 | N |
| ATOM | 1873 | CA | ALA | A | 261 | 13.400 | 7.789 | 43.320 | 1.00 | 18.68 | C |
| ATOM | 1874 | C | ALA | A | 261 | 13.326 | 6.472 | 44.100 | 1.00 | 18.95 | C |
| ATOM | 1875 | O | ALA | A | 261 | 13.216 | 5.402 | 43.503 | 1.00 | 18.96 | O |
| ATOM | 1876 | CB | ALA | A | 261 | 14.794 | 7.986 | 42.733 | 1.00 | 18.57 | C |
| ATOM | 1877 | N | ASP | A | 262 | 13.383 | 6.557 | 45.426 | 1.00 | 19.26 | N |
| ATOM | 1878 | CA | ASP | A | 262 | 13.374 | 5.371 | 46.278 | 1.00 | 19.74 | C |
| ATOM | 1879 | C | ASP | A | 262 | 11.964 | 4.836 | 46.560 | 1.00 | 19.82 | C |
| ATOM | 1880 | O | ASP | A | 262 | 11.804 | 3.704 | 47.028 | 1.00 | 19.80 | O |
| ATOM | 1881 | CB | ASP | A | 262 | 14.132 | 5.642 | 47.581 | 1.00 | 20.09 | C |
| ATOM | 1882 | CG | ASP | A | 262 | 15.614 | 5.901 | 47.351 | 1.00 | 21.02 | C |
| ATOM | 1883 | OD1 | ASP | A | 262 | 16.277 | 5.063 | 46.698 | 1.00 | 21.63 | O |
| ATOM | 1884 | OD2 | ASP | A | 262 | 16.204 | 6.917 | 47.780 | 1.00 | 22.09 | O |
| ATOM | 1885 | N | SER | A | 263 | 10.949 | 5.651 | 46.278 | 1.00 | 19.82 | N |
| ATOM | 1886 | CA | SER | A | 263 | 9.557 | 5.206 | 46.364 | 1.00 | 19.58 | C |
| ATOM | 1887 | C | SER | A | 263 | 9.039 | 4.767 | 44.995 | 1.00 | 19.43 | C |
| ATOM | 1888 | O | SER | A | 263 | 7.870 | 4.409 | 44.844 | 1.00 | 19.46 | O |
| ATOM | 1889 | CB | SER | A | 263 | 8.657 | 6.290 | 46.969 | 1.00 | 19.57 | C |
| ATOM | 1890 | OG | SER | A | 263 | 9.103 | 7.588 | 46.628 | 1.00 | 19.24 | O |
| ATOM | 1891 | N | ARG | A | 264 | 9.920 | 4.802 | 44.000 | 1.00 | 19.32 | N |
| ATOM | 1892 | CA | ARG | A | 264 | 9.621 | 4.260 | 42.682 | 1.00 | 19.28 | C |
| ATOM | 1893 | C | ARG | A | 264 | 9.760 | 2.744 | 42.752 | 1.00 | 19.36 | C |
| ATOM | 1894 | O | ARG | A | 264 | 10.562 | 2.241 | 43.541 | 1.00 | 19.44 | O |
| ATOM | 1895 | CB | ARG | A | 264 | 10.589 | 4.820 | 41.640 | 1.00 | 19.23 | C |
| ATOM | 1896 | CG | ARG | A | 264 | 10.261 | 6.214 | 41.140 | 1.00 | 18.85 | C |
| ATOM | 1897 | CD | ARG | A | 264 | 11.255 | 6.744 | 40.121 | 1.00 | 18.49 | C |
| ATOM | 1898 | NE | ARG | A | 264 | 11.374 | 8.199 | 40.175 | 1.00 | 18.10 | N |
| ATOM | 1899 | CZ | ARG | A | 264 | 12.469 | 8.880 | 39.860 | 1.00 | 18.13 | C |
| ATOM | 1900 | NH1 | ARG | A | 264 | 12.470 | 10.204 | 39.947 | 1.00 | 18.53 | N |
| ATOM | 1901 | NH2 | ARG | A | 264 | 13.565 | 8.250 | 39.461 | 1.00 | 17.66 | N |
| ATOM | 1902 | N | PRO | A | 265 | 8.986 | 2.015 | 41.946 | 1.00 | 19.45 | N |
| ATOM | 1903 | CA | PRO | A | 265 | 9.109 | 0.555 | 41.880 | 1.00 | 19.40 | C |
| ATOM | 1904 | C | PRO | A | 265 | 10.481 | 0.126 | 41.366 | 1.00 | 19.49 | C |
| ATOM | 1905 | O | PRO | A | 265 | 11.147 | 0.889 | 40.661 | 1.00 | 19.38 | O |
| ATOM | 1906 | CB | PRO | A | 265 | 8.035 | 0.159 | 40.863 | 1.00 | 19.41 | C |
| ATOM | 1907 | CG | PRO | A | 265 | 7.092 | 1.299 | 40.831 | 1.00 | 19.37 | C |
| ATOM | 1908 | CD | PRO | A | 265 | 7.933 | 2.513 | 41.042 | 1.00 | 19.62 | C |
| ATOM | 1909 | N | LYS | A | 266 | 10.902 | -1.076 | 41.741 | 1.00 | 19.55 | N |
| ATOM | 1910 | CA | LYS | A | 266 | 12.093 | -1.683 | 41.168 | 1.00 | 19.72 | C |
| ATOM | 1911 | C | LYS | A | 266 | 11.668 | -2.493 | 39.947 | 1.00 | 19.86 | C |
| ATOM | 1912 | O | LYS | A | 266 | 10.489 | -2.828 | 39.805 | 1.00 | 19.92 | O |
| ATOM | 1913 | CB | LYS | A | 266 | 12.794 | -2.570 | 42.197 | 1.00 | 19.77 | C |
| ATOM | 1914 | CG | LYS | A | 266 | 13.578 | -1.796 | 43.252 | 1.00 | 19.79 | C |
| ATOM | 1915 | N | PHE | A | 267 | 12.617 | -2.792 | 39.064 | 1.00 | 20.07 | N |

FIG. 4FF

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 1916 | CA | PHE | A | 267 | 12.329 | -3.570 | 37.858 | 1.00 | 20.25 | C |
| ATOM | 1917 | C | PHE | A | 267 | 11.921 | -5.004 | 38.184 | 1.00 | 20.45 | C |
| ATOM | 1918 | O | PHE | A | 267 | 11.101 | -5.592 | 37.477 | 1.00 | 20.54 | O |
| ATOM | 1919 | CB | PHE | A | 267 | 13.519 | -3.559 | 36.899 | 1.00 | 20.10 | C |
| ATOM | 1920 | CG | PHE | A | 267 | 13.692 | -2.261 | 36.159 | 1.00 | 20.16 | C |
| ATOM | 1921 | CD1 | PHE | A | 267 | 12.646 | -1.718 | 35.417 | 1.00 | 19.83 | C |
| ATOM | 1922 | CE1 | PHE | A | 267 | 12.806 | -0.521 | 34.734 | 1.00 | 19.70 | C |
| ATOM | 1923 | CZ | PHE | A | 267 | 14.022 | 0.144 | 34.784 | 1.00 | 19.60 | C |
| ATOM | 1924 | CE2 | PHE | A | 267 | 15.074 | -0.387 | 35.519 | 1.00 | 19.37 | C |
| ATOM | 1925 | CD2 | PHE | A | 267 | 14.907 | -1.581 | 36.200 | 1.00 | 19.75 | C |
| ATOM | 1926 | N | ARG | A | 268 | 12.493 | -5.549 | 39.256 | 1.00 | 20.64 | N |
| ATOM | 1927 | CA | ARG | A | 268 | 12.136 | -6.879 | 39.753 | 1.00 | 21.04 | C |
| ATOM | 1928 | C | ARG | A | 268 | 10.682 | -6.934 | 40.230 | 1.00 | 20.95 | C |
| ATOM | 1929 | O | ARG | A | 268 | 10.012 | -7.954 | 40.077 | 1.00 | 21.04 | O |
| ATOM | 1930 | CB | ARG | A | 268 | 13.094 | -7.327 | 40.871 | 1.00 | 21.21 | C |
| ATOM | 1931 | CG | ARG | A | 268 | 13.206 | -6.369 | 42.059 | 1.00 | 22.16 | C |
| ATOM | 1932 | CD | ARG | A | 268 | 13.475 | -7.044 | 43.399 | 1.00 | 23.52 | C |
| ATOM | 1933 | NE | ARG | A | 268 | 12.283 | -7.695 | 43.948 | 1.00 | 24.25 | N |
| ATOM | 1934 | CZ | ARG | A | 268 | 11.683 | -7.351 | 45.086 | 1.00 | 24.66 | C |
| ATOM | 1935 | NH1 | ARG | A | 268 | 10.605 | -8.012 | 45.487 | 1.00 | 24.72 | N |
| ATOM | 1936 | NH2 | ARG | A | 268 | 12.150 | -6.349 | 45.825 | 1.00 | 24.70 | N |
| ATOM | 1937 | N | GLU | A | 269 | 10.210 | -5.829 | 40.802 | 1.00 | 20.99 | N |
| ATOM | 1938 | CA | GLU | A | 269 | 8.831 | -5.702 | 41.259 | 1.00 | 21.07 | C |
| ATOM | 1939 | C | GLU | A | 269 | 7.869 | -5.607 | 40.082 | 1.00 | 20.97 | C |
| ATOM | 1940 | O | GLU | A | 269 | 6.783 | -6.190 | 40.113 | 1.00 | 20.98 | O |
| ATOM | 1941 | CB | GLU | A | 269 | 8.679 | -4.466 | 42.143 | 1.00 | 21.30 | C |
| ATOM | 1942 | CG | GLU | A | 269 | 8.849 | -4.734 | 43.626 | 1.00 | 22.18 | C |
| ATOM | 1943 | CD | GLU | A | 269 | 9.776 | -3.741 | 44.300 | 1.00 | 23.49 | C |
| ATOM | 1944 | OE1 | GLU | A | 269 | 9.790 | -2.556 | 43.891 | 1.00 | 23.93 | O |
| ATOM | 1945 | OE2 | GLU | A | 269 | 10.490 | -4.148 | 45.245 | 1.00 | 24.30 | O |
| ATOM | 1946 | N | LEU | A | 270 | 8.276 | -4.870 | 39.050 | 1.00 | 20.82 | N |
| ATOM | 1947 | CA | LEU | A | 270 | 7.459 | -4.681 | 37.854 | 1.00 | 20.61 | C |
| ATOM | 1948 | C | LEU | A | 270 | 7.276 | -5.980 | 37.066 | 1.00 | 20.44 | C |
| ATOM | 1949 | O | LEU | A | 270 | 6.268 | -6.147 | 36.380 | 1.00 | 20.53 | O |
| ATOM | 1950 | CB | LEU | A | 270 | 8.039 | -3.578 | 36.959 | 1.00 | 20.71 | C |
| ATOM | 1951 | CG | LEU | A | 270 | 8.118 | -2.152 | 37.527 | 1.00 | 20.96 | C |
| ATOM | 1952 | CD1 | LEU | A | 270 | 9.217 | -1.353 | 36.839 | 1.00 | 20.93 | C |
| ATOM | 1953 | CD2 | LEU | A | 270 | 6.787 | -1.418 | 37.427 | 1.00 | 20.87 | C |
| ATOM | 1954 | N | ILE | A | 271 | 8.247 | -6.890 | 37.170 | 1.00 | 20.18 | N |
| ATOM | 1955 | CA | ILE | A | 271 | 8.133 | -8.228 | 36.581 | 1.00 | 19.92 | C |
| ATOM | 1956 | C | ILE | A | 271 | 6.982 | -8.990 | 37.237 | 1.00 | 19.70 | C |
| ATOM | 1957 | O | ILE | A | 271 | 6.123 | -9.537 | 36.548 | 1.00 | 19.56 | O |
| ATOM | 1958 | CB | ILE | A | 271 | 9.464 | -9.031 | 36.715 | 1.00 | 19.98 | C |
| ATOM | 1959 | CG1 | ILE | A | 271 | 10.578 | -8.389 | 35.886 | 1.00 | 19.93 | C |
| ATOM | 1960 | CD1 | ILE | A | 271 | 11.972 | -8.724 | 36.371 | 1.00 | 19.76 | C |
| ATOM | 1961 | CG2 | ILE | A | 271 | 9.273 | -10.497 | 36.293 | 1.00 | 19.42 | C |
| ATOM | 1962 | N | ILE | A | 272 | 6.976 | -9.001 | 38.568 | 1.00 | 19.54 | N |
| ATOM | 1963 | CA | ILE | A | 272 | 5.958 | -9.693 | 39.356 | 1.00 | 19.56 | C |
| ATOM | 1964 | C | ILE | A | 272 | 4.554 | -9.131 | 39.111 | 1.00 | 19.55 | C |
| ATOM | 1965 | O | ILE | A | 272 | 3.623 | -9.886 | 38.830 | 1.00 | 19.71 | O |
| ATOM | 1966 | CB | ILE | A | 272 | 6.320 | -9.649 | 40.875 | 1.00 | 19.63 | C |
| ATOM | 1967 | CG1 | ILE | A | 272 | 7.697 | -10.290 | 41.147 | 1.00 | 19.53 | C |
| ATOM | 1968 | CD1 | ILE | A | 272 | 7.821 | -11.773 | 40.799 | 1.00 | 19.36 | C |
| ATOM | 1969 | CG2 | ILE | A | 272 | 5.199 | -10.254 | 41.743 | 1.00 | 19.53 | C |
| ATOM | 1970 | N | GLU | A | 273 | 4.416 | -7.810 | 39.205 | 1.00 | 19.52 | N |
| ATOM | 1971 | CA | GLU | A | 273 | 3.118 | -7.147 | 39.072 | 1.00 | 19.50 | C |
| ATOM | 1972 | C | GLU | A | 273 | 2.456 | -7.383 | 37.714 | 1.00 | 19.70 | C |
| ATOM | 1973 | O | GLU | A | 273 | 1.312 | -7.836 | 37.652 | 1.00 | 19.62 | O |
| ATOM | 1974 | CB | GLU | A | 273 | 3.249 | -5.647 | 39.345 | 1.00 | 19.34 | C |
| ATOM | 1975 | N | PHE | A | 274 | 3.186 | -7.085 | 36.638 | 1.00 | 19.92 | N |

FIG. 4GG

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 1976 | CA | PHE | A | 274 | 2.662 | -7.188 | 35.274 | 1.00 | 19.98 | C |
| ATOM | 1977 | C | PHE | A | 274 | 2.405 | -8.622 | 34.801 | 1.00 | 20.26 | C |
| ATOM | 1978 | O | PHE | A | 274 | 1.515 | -8.851 | 33.982 | 1.00 | 20.43 | O |
| ATOM | 1979 | CB | PHE | A | 274 | 3.586 | -6.470 | 34.285 | 1.00 | 19.73 | C |
| ATOM | 1980 | CG | PHE | A | 274 | 3.310 | -4.999 | 34.153 | 1.00 | 19.51 | C |
| ATOM | 1981 | CD1 | PHE | A | 274 | 2.072 | -4.543 | 33.711 | 1.00 | 19.39 | C |
| ATOM | 1982 | CE1 | PHE | A | 274 | 1.816 | -3.181 | 33.591 | 1.00 | 19.49 | C |
| ATOM | 1983 | CZ | PHE | A | 274 | 2.806 | -2.260 | 33.913 | 1.00 | 19.02 | C |
| ATOM | 1984 | CE2 | PHE | A | 274 | 4.045 | -2.706 | 34.354 | 1.00 | 18.83 | C |
| ATOM | 1985 | CD2 | PHE | A | 274 | 4.291 | -4.067 | 34.471 | 1.00 | 18.97 | C |
| ATOM | 1986 | N | SER | A | 275 | 3.186 | -9.579 | 35.300 | 1.00 | 20.63 | N |
| ATOM | 1987 | CA | SER | A | 275 | 2.982 | -10.986 | 34.945 | 1.00 | 21.17 | C |
| ATOM | 1988 | C | SER | A | 275 | 1.764 | -11.574 | 35.660 | 1.00 | 21.54 | C |
| ATOM | 1989 | O | SER | A | 275 | 1.128 | -12.501 | 35.149 | 1.00 | 21.55 | O |
| ATOM | 1990 | CB | SER | A | 275 | 4.235 | -11.818 | 35.221 | 1.00 | 20.92 | C |
| ATOM | 1991 | OG | SER | A | 275 | 4.554 | -11.809 | 36.596 | 1.00 | 21.07 | O |
| ATOM | 1992 | N | LYS | A | 276 | 1.454 | -11.030 | 36.838 | 1.00 | 22.01 | N |
| ATOM | 1993 | CA | LYS | A | 276 | 0.203 | -11.322 | 37.538 | 1.00 | 22.52 | C |
| ATOM | 1994 | C | LYS | A | 276 | -0.985 | -10.798 | 36.731 | 1.00 | 22.84 | C |
| ATOM | 1995 | O | LYS | A | 276 | -2.021 | -11.459 | 36.632 | 1.00 | 23.00 | O |
| ATOM | 1996 | CB | LYS | A | 276 | 0.203 | -10.689 | 38.931 | 1.00 | 22.47 | C |
| ATOM | 1997 | CG | LYS | A | 276 | 0.871 | -11.533 | 39.997 | 1.00 | 23.00 | C |
| ATOM | 1998 | CD | LYS | A | 276 | 1.188 | -10.716 | 41.237 | 1.00 | 23.49 | C |
| ATOM | 1999 | CE | LYS | A | 276 | 1.590 | -11.615 | 42.394 | 1.00 | 23.73 | C |
| ATOM | 2000 | NZ | LYS | A | 276 | 2.144 | -10.839 | 43.539 | 1.00 | 24.02 | N |
| ATOM | 2001 | N | MET | A | 277 | -0.816 | -9.609 | 36.154 | 1.00 | 23.18 | N |
| ATOM | 2002 | CA | MET | A | 277 | -1.831 | -8.988 | 35.308 | 1.00 | 23.62 | C |
| ATOM | 2003 | C | MET | A | 277 | -1.952 | -9.696 | 33.959 | 1.00 | 23.92 | C |
| ATOM | 2004 | O | MET | A | 277 | -3.026 | -9.717 | 33.360 | 1.00 | 23.88 | O |
| ATOM | 2005 | CB | MET | A | 277 | -1.526 | -7.501 | 35.103 | 1.00 | 23.54 | C |
| ATOM | 2006 | CG | MET | A | 277 | -1.647 | -6.654 | 36.366 | 1.00 | 23.73 | C |
| ATOM | 2007 | SD | MET | A | 277 | -1.239 | -4.919 | 36.090 | 1.00 | 23.64 | S |
| ATOM | 2008 | CE | MET | A | 277 | -1.698 | -4.208 | 37.645 | 1.00 | 23.72 | C |
| ATOM | 2009 | N | ALA | A | 278 | -0.845 | -10.268 | 33.489 | 1.00 | 24.44 | N |
| ATOM | 2010 | CA | ALA | A | 278 | -0.821 | -11.034 | 32.240 | 1.00 | 24.93 | C |
| ATOM | 2011 | C | ALA | A | 278 | -1.600 | -12.348 | 32.353 | 1.00 | 25.26 | C |
| ATOM | 2012 | O | ALA | A | 278 | -2.041 | -12.901 | 31.344 | 1.00 | 25.34 | O |
| ATOM | 2013 | CB | ALA | A | 278 | 0.614 | -11.299 | 31.804 | 1.00 | 24.73 | C |
| ATOM | 2014 | N | ARG | A | 279 | -1.766 | -12.837 | 33.581 | 1.00 | 25.71 | N |
| ATOM | 2015 | CA | ARG | A | 279 | -2.548 | -14.043 | 33.847 | 1.00 | 26.32 | C |
| ATOM | 2016 | C | ARG | A | 279 | -4.062 | -13.809 | 33.737 | 1.00 | 26.68 | C |
| ATOM | 2017 | O | ARG | A | 279 | -4.822 | -14.748 | 33.492 | 1.00 | 26.80 | O |
| ATOM | 2018 | CB | ARG | A | 279 | -2.192 | -14.619 | 35.222 | 1.00 | 26.38 | C |
| ATOM | 2019 | CG | ARG | A | 279 | -0.915 | -15.453 | 35.231 | 1.00 | 26.37 | C |
| ATOM | 2020 | CD | ARG | A | 279 | -0.292 | -15.630 | 36.604 | 1.00 | 25.96 | C |
| ATOM | 2021 | N | ASP | A | 280 | -4.484 | -12.559 | 33.926 | 1.00 | 27.14 | N |
| ATOM | 2022 | CA | ASP | A | 280 | -5.885 | -12.158 | 33.796 | 1.00 | 27.50 | C |
| ATOM | 2023 | C | ASP | A | 280 | -5.966 | -10.837 | 33.021 | 1.00 | 27.75 | C |
| ATOM | 2024 | O | ASP | A | 280 | -6.248 | -9.786 | 33.605 | 1.00 | 27.91 | O |
| ATOM | 2025 | CB | ASP | A | 280 | -6.523 | -12.006 | 35.182 | 1.00 | 27.63 | C |
| ATOM | 2026 | CG | ASP | A | 280 | -8.025 | -12.247 | 35.174 | 1.00 | 28.04 | C |
| ATOM | 2027 | OD1 | ASP | A | 280 | -8.734 | -11.648 | 34.338 | 1.00 | 28.59 | O |
| ATOM | 2028 | OD2 | ASP | A | 280 | -8.590 | -13.015 | 35.980 | 1.00 | 28.47 | O |
| ATOM | 2029 | N | PRO | A | 281 | -5.729 | -10.895 | 31.709 | 1.00 | 27.81 | N |
| ATOM | 2030 | CA | PRO | A | 281 | -5.502 | -9.690 | 30.895 | 1.00 | 27.88 | C |
| ATOM | 2031 | C | PRO | A | 281 | -6.682 | -8.719 | 30.823 | 1.00 | 28.00 | C |
| ATOM | 2032 | O | PRO | A | 281 | -6.471 | -7.508 | 30.918 | 1.00 | 27.90 | O |
| ATOM | 2033 | CB | PRO | A | 281 | -5.204 | -10.258 | 29.502 | 1.00 | 27.85 | C |
| ATOM | 2034 | CG | PRO | A | 281 | -4.835 | -11.674 | 29.739 | 1.00 | 27.90 | C |
| ATOM | 2035 | CD | PRO | A | 281 | -5.669 | -12.121 | 30.894 | 1.00 | 27.81 | C |

FIG. 4HH

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|---------|---------|--------|------|-------|---|
| ATOM | 2036 | N | GLN | A | 282 | -7.895 | -9.244 | 30.659 | 1.00 | 28.19 | N |
| ATOM | 2037 | CA | GLN | A | 282 | -9.088 | -8.413 | 30.492 | 1.00 | 28.23 | C |
| ATOM | 2038 | C | GLN | A | 282 | -9.601 | -7.824 | 31.812 | 1.00 | 28.18 | C |
| ATOM | 2039 | O | GLN | A | 282 | -10.509 | -6.990 | 31.816 | 1.00 | 28.24 | O |
| ATOM | 2040 | CB | GLN | A | 282 | -10.187 | -9.195 | 29.765 | 1.00 | 28.37 | C |
| ATOM | 2041 | CG | GLN | A | 282 | -9.932 | -9.339 | 28.268 | 1.00 | 29.06 | C |
| ATOM | 2042 | CD | GLN | A | 282 | -10.875 | -10.312 | 27.589 | 1.00 | 29.88 | C |
| ATOM | 2043 | OE1 | GLN | A | 282 | -12.044 | -9.995 | 27.358 | 1.00 | 30.65 | O |
| ATOM | 2044 | NE2 | GLN | A | 282 | -10.368 | -11.494 | 27.256 | 1.00 | 29.87 | N |
| ATOM | 2045 | N | ARG | A | 283 | -9.011 | -8.257 | 32.923 | 1.00 | 28.06 | N |
| ATOM | 2046 | CA | ARG | A | 283 | -9.304 | -7.690 | 34.235 | 1.00 | 28.09 | C |
| ATOM | 2047 | C | ARG | A | 283 | -8.652 | -6.317 | 34.387 | 1.00 | 27.94 | C |
| ATOM | 2048 | O | ARG | A | 283 | -9.215 | -5.415 | 35.010 | 1.00 | 27.90 | O |
| ATOM | 2049 | CB | ARG | A | 283 | -8.808 | -8.627 | 35.343 | 1.00 | 28.28 | C |
| ATOM | 2050 | CG | ARG | A | 283 | -9.257 | -8.252 | 36.752 | 1.00 | 28.68 | C |
| ATOM | 2051 | CD | ARG | A | 283 | -8.664 | -9.127 | 37.844 | 1.00 | 29.47 | C |
| ATOM | 2052 | NE | ARG | A | 283 | -8.775 | -8.510 | 39.165 | 1.00 | 30.16 | N |
| ATOM | 2053 | CZ | ARG | A | 283 | -8.645 | -9.161 | 40.318 | 1.00 | 30.73 | C |
| ATOM | 2054 | NH1 | ARG | A | 283 | -8.394 | -10.467 | 40.333 | 1.00 | 30.92 | N |
| ATOM | 2055 | NH2 | ARG | A | 283 | -8.767 | -8.505 | 41.465 | 1.00 | 30.86 | N |
| ATOM | 2056 | N | TYR | A | 284 | -7.465 | -6.171 | 33.806 | 1.00 | 27.76 | N |
| ATOM | 2057 | CA | TYR | A | 284 | -6.640 | -4.989 | 34.024 | 1.00 | 27.59 | C |
| ATOM | 2058 | C | TYR | A | 284 | -6.608 | -4.036 | 32.831 | 1.00 | 27.61 | C |
| ATOM | 2059 | O | TYR | A | 284 | -6.302 | -2.853 | 32.990 | 1.00 | 27.37 | O |
| ATOM | 2060 | CB | TYR | A | 284 | -5.226 | -5.405 | 34.432 | 1.00 | 27.46 | C |
| ATOM | 2061 | CG | TYR | A | 284 | -5.177 | -6.173 | 35.735 | 1.00 | 27.33 | C |
| ATOM | 2062 | CD1 | TYR | A | 284 | -5.194 | -7.568 | 35.744 | 1.00 | 27.09 | C |
| ATOM | 2063 | CE1 | TYR | A | 284 | -5.150 | -8.280 | 36.936 | 1.00 | 26.78 | C |
| ATOM | 2064 | CZ | TYR | A | 284 | -5.093 | -7.595 | 38.136 | 1.00 | 26.76 | C |
| ATOM | 2065 | OH | TYR | A | 284 | -5.051 | -8.299 | 39.315 | 1.00 | 26.68 | O |
| ATOM | 2066 | CE2 | TYR | A | 284 | -5.078 | -6.209 | 38.157 | 1.00 | 26.83 | C |
| ATOM | 2067 | CD2 | TYR | A | 284 | -5.121 | -5.506 | 36.960 | 1.00 | 27.00 | C |
| ATOM | 2068 | N | LEU | A | 285 | -6.924 | -4.552 | 31.645 | 1.00 | 27.69 | N |
| ATOM | 2069 | CA | LEU | A | 285 | -7.037 | -3.721 | 30.449 | 1.00 | 27.89 | C |
| ATOM | 2070 | C | LEU | A | 285 | -8.373 | -3.941 | 29.751 | 1.00 | 28.17 | C |
| ATOM | 2071 | O | LEU | A | 285 | -8.772 | -5.081 | 29.506 | 1.00 | 28.31 | O |
| ATOM | 2072 | CB | LEU | A | 285 | -5.876 | -3.975 | 29.480 | 1.00 | 27.76 | C |
| ATOM | 2073 | CG | LEU | A | 285 | -4.447 | -3.602 | 29.900 | 1.00 | 27.57 | C |
| ATOM | 2074 | CD1 | LEU | A | 285 | -3.470 | -3.959 | 28.794 | 1.00 | 27.30 | C |
| ATOM | 2075 | CD2 | LEU | A | 285 | -4.314 | -2.125 | 30.277 | 1.00 | 27.55 | C |
| ATOM | 2076 | N | VAL | A | 286 | -9.058 | -2.844 | 29.437 | 1.00 | 28.61 | N |
| ATOM | 2077 | CA | VAL | A | 286 | -10.371 | -2.903 | 28.792 | 1.00 | 28.82 | C |
| ATOM | 2078 | C | VAL | A | 286 | -10.282 | -2.511 | 27.314 | 1.00 | 29.03 | C |
| ATOM | 2079 | O | VAL | A | 286 | -10.167 | -1.331 | 26.972 | 1.00 | 29.00 | O |
| ATOM | 2080 | CB | VAL | A | 286 | -11.425 | -2.038 | 29.539 | 1.00 | 28.82 | C |
| ATOM | 2081 | CG1 | VAL | A | 286 | -12.804 | -2.183 | 28.900 | 1.00 | 28.77 | C |
| ATOM | 2082 | CG2 | VAL | A | 286 | -11.481 | -2.417 | 31.016 | 1.00 | 28.38 | C |
| ATOM | 2083 | N | ILE | A | 287 | -10.331 | -3.522 | 26.452 | 1.00 | 29.44 | N |
| ATOM | 2084 | CA | ILE | A | 287 | -10.239 | -3.340 | 25.005 | 1.00 | 29.87 | C |
| ATOM | 2085 | C | ILE | A | 287 | -11.505 | -3.880 | 24.332 | 1.00 | 30.08 | C |
| ATOM | 2086 | O | ILE | A | 287 | -12.022 | -4.929 | 24.724 | 1.00 | 30.14 | O |
| ATOM | 2087 | CB | ILE | A | 287 | -8.960 | -4.036 | 24.463 | 1.00 | 29.91 | C |
| ATOM | 2088 | CG1 | ILE | A | 287 | -7.716 | -3.229 | 24.842 | 1.00 | 30.14 | C |
| ATOM | 2089 | CD1 | ILE | A | 287 | -6.609 | -4.059 | 25.452 | 1.00 | 30.12 | C |
| ATOM | 2090 | CG2 | ILE | A | 287 | -9.014 | -4.227 | 22.949 | 1.00 | 30.04 | C |
| ATOM | 2091 | N | GLN | A | 288 | -11.996 | -3.147 | 23.330 | 1.00 | 30.42 | N |
| ATOM | 2092 | CA | GLN | A | 288 | -13.221 | -3.495 | 22.605 | 1.00 | 30.66 | C |
| ATOM | 2093 | C | GLN | A | 288 | -13.100 | -4.820 | 21.847 | 1.00 | 30.64 | C |
| ATOM | 2094 | O | GLN | A | 288 | -12.458 | -4.898 | 20.796 | 1.00 | 30.62 | O |
| ATOM | 2095 | CB | GLN | A | 288 | -13.610 | -2.370 | 21.638 | 1.00 | 30.72 | C |

FIG. 4II

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|---------|--------|---------|------|-------|---|
| ATOM | 2096 | CG | GLN | A | 288 | -14.354 | -1.206 | 22.280 | 1.00 | 31.26 | C |
| ATOM | 2097 | CD | GLN | A | 288 | -14.691 | -0.101 | 21.286 | 1.00 | 32.11 | C |
| ATOM | 2098 | OE1 | GLN | A | 288 | -15.299 | -0.355 | 20.242 | 1.00 | 32.33 | O |
| ATOM | 2099 | NE2 | GLN | A | 288 | -14.301 | 1.126 | 21.610 | 1.00 | 32.21 | N |
| TER | 2100 | | GLN | A | 288 | | | | | | |
| ATOM | 2101 | N | LEU | B | 9 | 47.691 | 6.198 | 5.619 | 1.00 | 33.98 | N |
| ATOM | 2102 | CA | LEU | B | 9 | 49.166 | 6.110 | 5.822 | 1.00 | 34.01 | C |
| ATOM | 2103 | C | LEU | B | 9 | 49.937 | 7.098 | 4.952 | 1.00 | 33.88 | C |
| ATOM | 2104 | O | LEU | B | 9 | 49.419 | 7.605 | 3.955 | 1.00 | 33.80 | O |
| ATOM | 2105 | CB | LEU | B | 9 | 49.665 | 4.687 | 5.554 | 1.00 | 34.13 | C |
| ATOM | 2106 | CG | LEU | B | 9 | 50.103 | 3.870 | 6.774 | 1.00 | 34.26 | C |
| ATOM | 2107 | CD1 | LEU | B | 9 | 49.775 | 2.399 | 6.561 | 1.00 | 34.63 | C |
| ATOM | 2108 | CD2 | LEU | B | 9 | 51.587 | 4.057 | 7.066 | 1.00 | 33.89 | C |
| ATOM | 2109 | N | LEU | B | 10 | 51.181 | 7.355 | 5.347 | 1.00 | 33.81 | N |
| ATOM | 2110 | CA | LEU | B | 10 | 52.079 | 8.246 | 4.622 | 1.00 | 33.84 | C |
| ATOM | 2111 | C | LEU | B | 10 | 52.528 | 7.636 | 3.297 | 1.00 | 33.93 | C |
| ATOM | 2112 | O | LEU | B | 10 | 52.716 | 6.421 | 3.189 | 1.00 | 33.83 | O |
| ATOM | 2113 | CB | LEU | B | 10 | 53.294 | 8.585 | 5.494 | 1.00 | 33.78 | C |
| ATOM | 2114 | CG | LEU | B | 10 | 54.397 | 9.519 | 4.982 | 1.00 | 33.65 | C |
| ATOM | 2115 | CD1 | LEU | B | 10 | 53.948 | 10.973 | 4.961 | 1.00 | 33.13 | C |
| ATOM | 2116 | CD2 | LEU | B | 10 | 55.644 | 9.353 | 5.835 | 1.00 | 33.69 | C |
| ATOM | 2117 | N | ARG | B | 11 | 52.684 | 8.497 | 2.295 | 1.00 | 34.00 | N |
| ATOM | 2118 | CA | ARG | B | 11 | 53.220 | 8.103 | 0.998 | 1.00 | 34.04 | C |
| ATOM | 2119 | C | ARG | B | 11 | 54.595 | 8.736 | 0.796 | 1.00 | 34.14 | C |
| ATOM | 2120 | O | ARG | B | 11 | 54.713 | 9.955 | 0.643 | 1.00 | 34.14 | O |
| ATOM | 2121 | CB | ARG | B | 11 | 52.272 | 8.525 | -0.130 | 1.00 | 34.00 | C |
| ATOM | 2122 | CG | ARG | B | 11 | 51.030 | 7.660 | -0.270 | 1.00 | 34.10 | C |
| ATOM | 2123 | N | ILE | B | 12 | 55.636 | 7.909 | 0.824 | 1.00 | 34.28 | N |
| ATOM | 2124 | CA | ILE | B | 12 | 56.974 | 8.368 | 0.474 | 1.00 | 34.31 | C |
| ATOM | 2125 | C | ILE | B | 12 | 57.011 | 8.499 | -1.042 | 1.00 | 34.41 | C |
| ATOM | 2126 | O | ILE | B | 12 | 56.900 | 7.505 | -1.768 | 1.00 | 34.55 | O |
| ATOM | 2127 | CB | ILE | B | 12 | 58.066 | 7.393 | 0.978 | 1.00 | 34.30 | C |
| ATOM | 2128 | CG1 | ILE | B | 12 | 57.908 | 7.121 | 2.476 | 1.00 | 34.45 | C |
| ATOM | 2129 | CD1 | ILE | B | 12 | 58.011 | 5.655 | 2.848 | 1.00 | 34.43 | C |
| ATOM | 2130 | CG2 | ILE | B | 12 | 59.454 | 7.956 | 0.696 | 1.00 | 34.38 | C |
| ATOM | 2131 | N | LEU | B | 13 | 57.143 | 9.734 | -1.513 | 1.00 | 34.36 | N |
| ATOM | 2132 | CA | LEU | B | 13 | 57.074 | 10.018 | -2.939 | 1.00 | 34.39 | C |
| ATOM | 2133 | C | LEU | B | 13 | 58.438 | 10.338 | -3.529 | 1.00 | 34.49 | C |
| ATOM | 2134 | O | LEU | B | 13 | 59.251 | 11.022 | -2.904 | 1.00 | 34.59 | O |
| ATOM | 2135 | CB | LEU | B | 13 | 56.094 | 11.167 | -3.216 | 1.00 | 34.31 | C |
| ATOM | 2136 | CG | LEU | B | 13 | 54.677 | 11.094 | -2.629 | 1.00 | 34.02 | C |
| ATOM | 2137 | CD1 | LEU | B | 13 | 53.957 | 12.412 | -2.843 | 1.00 | 33.52 | C |
| ATOM | 2138 | CD2 | LEU | B | 13 | 53.872 | 9.945 | -3.226 | 1.00 | 33.81 | C |
| ATOM | 2139 | N | LYS | B | 14 | 58.679 | 9.831 | -4.735 | 1.00 | 34.55 | N |
| ATOM | 2140 | CA | LYS | B | 14 | 59.860 | 10.193 | -5.511 | 1.00 | 34.65 | C |
| ATOM | 2141 | C | LYS | B | 14 | 59.681 | 11.616 | -6.028 | 1.00 | 34.79 | C |
| ATOM | 2142 | O | LYS | B | 14 | 58.549 | 12.055 | -6.258 | 1.00 | 34.91 | O |
| ATOM | 2143 | CB | LYS | B | 14 | 60.048 | 9.229 | -6.686 | 1.00 | 34.65 | C |
| ATOM | 2144 | CG | LYS | B | 14 | 60.455 | 7.815 | -6.286 | 1.00 | 34.45 | C |
| ATOM | 2145 | N | GLU | B | 15 | 60.790 | 12.332 | -6.209 | 1.00 | 34.75 | N |
| ATOM | 2146 | CA | GLU | B | 15 | 60.753 | 13.705 | -6.722 | 1.00 | 34.75 | C |
| ATOM | 2147 | C | GLU | B | 15 | 60.186 | 13.779 | -8.145 | 1.00 | 34.70 | C |
| ATOM | 2148 | O | GLU | B | 15 | 59.829 | 14.858 | -8.625 | 1.00 | 34.80 | O |
| ATOM | 2149 | CB | GLU | B | 15 | 62.145 | 14.342 | -6.670 | 1.00 | 34.73 | C |
| ATOM | 2150 | N | THR | B | 16 | 60.095 | 12.624 | -8.798 | 1.00 | 34.65 | N |
| ATOM | 2151 | CA | THR | B | 16 | 59.594 | 12.524 | -10.167 | 1.00 | 34.59 | C |
| ATOM | 2152 | C | THR | B | 16 | 58.074 | 12.325 | -10.245 | 1.00 | 34.36 | C |
| ATOM | 2153 | O | THR | B | 16 | 57.500 | 12.303 | -11.337 | 1.00 | 34.30 | O |
| ATOM | 2154 | CB | THR | B | 16 | 60.346 | 11.399 | -10.932 | 1.00 | 34.67 | C |
| ATOM | 2155 | OG1 | THR | B | 16 | 60.009 | 11.452 | -12.324 | 1.00 | 35.10 | O |

FIG. 4JJ

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|---------|------|-------|---|
| ATOM | 2156 | CG2 | THR | B | 16 | 59.868 | 10.011 | -10.494 | 1.00 | 34.46 | C |
| ATOM | 2157 | N | GLU | B | 17 | 57.431 | 12.182 | -9.087 | 1.00 | 34.13 | N |
| ATOM | 2158 | CA | GLU | B | 17 | 55.993 | 11.911 | -9.028 | 1.00 | 33.82 | C |
| ATOM | 2159 | C | GLU | B | 17 | 55.158 | 13.170 | -8.777 | 1.00 | 33.45 | C |
| ATOM | 2160 | O | GLU | B | 17 | 53.932 | 13.099 | -8.687 | 1.00 | 33.43 | O |
| ATOM | 2161 | CB | GLU | B | 17 | 55.686 | 10.840 | -7.974 | 1.00 | 33.93 | C |
| ATOM | 2162 | CG | GLU | B | 17 | 56.287 | 9.475 | -8.280 | 1.00 | 34.40 | C |
| ATOM | 2163 | CD | GLU | B | 17 | 55.885 | 8.410 | -7.278 | 1.00 | 34.89 | C |
| ATOM | 2164 | OE1 | GLU | B | 17 | 56.253 | 8.529 | -6.088 | 1.00 | 35.15 | O |
| ATOM | 2165 | OE2 | GLU | B | 17 | 55.203 | 7.446 | -7.684 | 1.00 | 35.28 | O |
| ATOM | 2166 | N | PHE | B | 18 | 55.826 | 14.316 | -8.669 | 1.00 | 33.09 | N |
| ATOM | 2167 | CA | PHE | B | 18 | 55.151 | 15.596 | -8.459 | 1.00 | 32.70 | C |
| ATOM | 2168 | C | PHE | B | 18 | 55.930 | 16.763 | -9.065 | 1.00 | 32.51 | C |
| ATOM | 2169 | O | PHE | B | 18 | 57.148 | 16.684 | -9.224 | 1.00 | 32.58 | O |
| ATOM | 2170 | CB | PHE | B | 18 | 54.882 | 15.837 | -6.964 | 1.00 | 32.63 | C |
| ATOM | 2171 | CG | PHE | B | 18 | 56.125 | 16.021 | -6.137 | 1.00 | 32.22 | C |
| ATOM | 2172 | CD1 | PHE | B | 18 | 56.610 | 17.296 | -5.862 | 1.00 | 32.20 | C |
| ATOM | 2173 | CE1 | PHE | B | 18 | 57.758 | 17.473 | -5.095 | 1.00 | 32.34 | C |
| ATOM | 2174 | CZ | PHE | B | 18 | 58.430 | 16.367 | -4.590 | 1.00 | 32.41 | C |
| ATOM | 2175 | CE2 | PHE | B | 18 | 57.950 | 15.088 | -4.855 | 1.00 | 32.46 | C |
| ATOM | 2176 | CD2 | PHE | B | 18 | 56.800 | 14.923 | -5.620 | 1.00 | 32.23 | C |
| ATOM | 2177 | N | LYS | B | 19 | 55.218 | 17.839 | -9.394 | 1.00 | 32.35 | N |
| ATOM | 2178 | CA | LYS | B | 19 | 55.825 | 19.045 | -9.957 | 1.00 | 32.30 | C |
| ATOM | 2179 | C | LYS | B | 19 | 55.187 | 20.314 | -9.389 | 1.00 | 32.32 | C |
| ATOM | 2180 | O | LYS | B | 19 | 53.969 | 20.382 | -9.220 | 1.00 | 32.35 | O |
| ATOM | 2181 | CB | LYS | B | 19 | 55.709 | 19.037 | -11.484 | 1.00 | 32.28 | C |
| ATOM | 2182 | CG | LYS | B | 19 | 56.712 | 19.932 | -12.198 | 1.00 | 32.23 | C |
| ATOM | 2183 | N | LYS | B | 20 | 56.021 | 21.311 | -9.100 | 1.00 | 32.26 | N |
| ATOM | 2184 | CA | LYS | B | 20 | 55.560 | 22.590 | -8.564 | 1.00 | 32.30 | C |
| ATOM | 2185 | C | LYS | B | 20 | 55.272 | 23.570 | -9.701 | 1.00 | 32.30 | C |
| ATOM | 2186 | O | LYS | B | 20 | 56.129 | 23.809 | -10.554 | 1.00 | 32.41 | O |
| ATOM | 2187 | CB | LYS | B | 20 | 56.595 | 23.178 | -7.597 | 1.00 | 32.35 | C |
| ATOM | 2188 | CG | LYS | B | 20 | 57.022 | 22.234 | -6.471 | 1.00 | 32.35 | C |
| ATOM | 2189 | CD | LYS | B | 20 | 58.145 | 22.825 | -5.622 | 1.00 | 32.48 | C |
| ATOM | 2190 | CE | LYS | B | 20 | 59.525 | 22.510 | -6.199 | 1.00 | 32.80 | C |
| ATOM | 2191 | NZ | LYS | B | 20 | 59.966 | 21.116 | -5.913 | 1.00 | 32.82 | N |
| ATOM | 2192 | N | ILE | B | 21 | 54.066 | 24.136 | -9.705 | 1.00 | 32.17 | N |
| ATOM | 2193 | CA | ILE | B | 21 | 53.602 | 24.971 | -10.814 | 1.00 | 31.94 | C |
| ATOM | 2194 | C | ILE | B | 21 | 53.524 | 26.455 | -10.447 | 1.00 | 31.94 | C |
| ATOM | 2195 | O | ILE | B | 21 | 54.124 | 27.294 | -11.118 | 1.00 | 32.04 | O |
| ATOM | 2196 | CB | ILE | B | 21 | 52.247 | 24.437 | -11.366 | 1.00 | 31.98 | C |
| ATOM | 2197 | CG1 | ILE | B | 21 | 52.463 | 23.112 | -12.103 | 1.00 | 32.04 | C |
| ATOM | 2198 | CD1 | ILE | B | 21 | 51.503 | 22.019 | -11.708 | 1.00 | 32.21 | C |
| ATOM | 2199 | CG2 | ILE | B | 21 | 51.582 | 25.450 | -12.300 | 1.00 | 31.74 | C |
| ATOM | 2200 | N | LYS | B | 22 | 52.787 | 26.775 | -9.388 | 1.00 | 31.85 | N |
| ATOM | 2201 | CA | LYS | B | 22 | 52.634 | 28.162 | -8.961 | 1.00 | 31.71 | C |
| ATOM | 2202 | C | LYS | B | 22 | 53.041 | 28.335 | -7.506 | 1.00 | 31.60 | C |
| ATOM | 2203 | O | LYS | B | 22 | 52.793 | 27.457 | -6.682 | 1.00 | 31.69 | O |
| ATOM | 2204 | CB | LYS | B | 22 | 51.191 | 28.630 | -9.162 | 1.00 | 31.79 | C |
| ATOM | 2205 | N | VAL | B | 23 | 53.676 | 29.464 | -7.200 | 1.00 | 31.28 | N |
| ATOM | 2206 | CA | VAL | B | 23 | 54.018 | 29.800 | -5.822 | 1.00 | 31.08 | C |
| ATOM | 2207 | C | VAL | B | 23 | 52.773 | 30.362 | -5.149 | 1.00 | 30.96 | C |
| ATOM | 2208 | O | VAL | B | 23 | 52.146 | 31.289 | -5.668 | 1.00 | 31.13 | O |
| ATOM | 2209 | CB | VAL | B | 23 | 55.188 | 30.826 | -5.739 | 1.00 | 31.10 | C |
| ATOM | 2210 | CG1 | VAL | B | 23 | 55.499 | 31.199 | -4.291 | 1.00 | 30.73 | C |
| ATOM | 2211 | CG2 | VAL | B | 23 | 56.439 | 30.284 | -6.418 | 1.00 | 31.48 | C |
| ATOM | 2212 | N | LEU | B | 24 | 52.403 | 29.789 | -4.008 | 1.00 | 30.68 | N |
| ATOM | 2213 | CA | LEU | B | 24 | 51.286 | 30.317 | -3.230 | 1.00 | 30.58 | C |
| ATOM | 2214 | C | LEU | B | 24 | 51.762 | 31.423 | -2.294 | 1.00 | 30.48 | C |
| ATOM | 2215 | O | LEU | B | 24 | 51.081 | 32.435 | -2.119 | 1.00 | 30.46 | O |

FIG. 4KK

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2216 | CB | LEU | B | 24 | 50.579 | 29.206 | -2.448 | 1.00 | 30.42 | C |
| ATOM | 2217 | CG | LEU | B | 24 | 49.328 | 28.610 | -3.104 | 1.00 | 30.39 | C |
| ATOM | 2218 | CD1 | LEU | B | 24 | 49.100 | 27.189 | -2.620 | 1.00 | 30.63 | C |
| ATOM | 2219 | CD2 | LEU | B | 24 | 48.094 | 29.468 | -2.837 | 1.00 | 30.36 | C |
| ATOM | 2220 | N | GLY | B | 25 | 52.941 | 31.225 | -1.708 | 1.00 | 30.43 | N |
| ATOM | 2221 | CA | GLY | B | 25 | 53.526 | 32.188 | -0.793 | 1.00 | 30.28 | C |
| ATOM | 2222 | C | GLY | B | 25 | 54.471 | 31.553 | 0.209 | 1.00 | 30.30 | C |
| ATOM | 2223 | O | GLY | B | 25 | 54.652 | 30.331 | 0.229 | 1.00 | 30.17 | O |
| ATOM | 2224 | N | SER | B | 26 | 55.070 | 32.397 | 1.047 | 1.00 | 30.26 | N |
| ATOM | 2225 | CA | SER | B | 26 | 56.030 | 31.959 | 2.055 | 1.00 | 30.20 | C |
| ATOM | 2226 | C | SER | B | 26 | 55.515 | 32.225 | 3.468 | 1.00 | 30.14 | C |
| ATOM | 2227 | O | SER | B | 26 | 54.572 | 32.992 | 3.660 | 1.00 | 30.35 | O |
| ATOM | 2228 | CB | SER | B | 26 | 57.371 | 32.662 | 1.845 | 1.00 | 30.13 | C |
| ATOM | 2229 | OG | SER | B | 26 | 57.783 | 32.574 | 0.494 | 1.00 | 30.57 | O |
| ATOM | 2230 | N | GLY | B | 27 | 56.140 | 31.583 | 4.450 | 1.00 | 30.06 | N |
| ATOM | 2231 | CA | GLY | B | 27 | 55.783 | 31.766 | 5.844 | 1.00 | 29.95 | C |
| ATOM | 2232 | C | GLY | B | 27 | 56.990 | 31.765 | 6.762 | 1.00 | 29.94 | C |
| ATOM | 2233 | O | GLY | B | 27 | 58.023 | 32.365 | 6.451 | 1.00 | 30.05 | O |
| ATOM | 2234 | N | ALA | B | 28 | 56.853 | 31.088 | 7.897 | 1.00 | 29.79 | N |
| ATOM | 2235 | CA | ALA | B | 28 | 57.906 | 31.024 | 8.904 | 1.00 | 29.69 | C |
| ATOM | 2236 | C | ALA | B | 28 | 58.713 | 29.732 | 8.817 | 1.00 | 29.66 | C |
| ATOM | 2237 | O | ALA | B | 28 | 59.796 | 29.638 | 9.390 | 1.00 | 29.72 | O |
| ATOM | 2238 | CB | ALA | B | 28 | 57.314 | 31.187 | 10.300 | 1.00 | 29.53 | C |
| ATOM | 2239 | N | PHE | B | 29 | 58.184 | 28.745 | 8.094 | 1.00 | 29.64 | N |
| ATOM | 2240 | CA | PHE | B | 29 | 58.789 | 27.415 | 8.033 | 1.00 | 29.41 | C |
| ATOM | 2241 | C | PHE | B | 29 | 59.009 | 26.908 | 6.611 | 1.00 | 29.33 | C |
| ATOM | 2242 | O | PHE | B | 29 | 59.776 | 25.964 | 6.399 | 1.00 | 29.49 | O |
| ATOM | 2243 | CB | PHE | B | 29 | 57.940 | 26.406 | 8.814 | 1.00 | 29.42 | C |
| ATOM | 2244 | CG | PHE | B | 29 | 57.887 | 26.673 | 10.289 | 1.00 | 29.64 | C |
| ATOM | 2245 | CD1 | PHE | B | 29 | 58.971 | 26.366 | 11.104 | 1.00 | 29.76 | C |
| ATOM | 2246 | CE1 | PHE | B | 29 | 58.925 | 26.619 | 12.470 | 1.00 | 30.09 | C |
| ATOM | 2247 | CZ | PHE | B | 29 | 57.784 | 27.184 | 13.034 | 1.00 | 29.98 | C |
| ATOM | 2248 | CE2 | PHE | B | 29 | 56.696 | 27.493 | 12.229 | 1.00 | 29.75 | C |
| ATOM | 2249 | CD2 | PHE | B | 29 | 56.752 | 27.237 | 10.863 | 1.00 | 29.79 | C |
| ATOM | 2250 | N | GLY | B | 30 | 58.336 | 27.520 | 5.641 | 1.00 | 29.09 | N |
| ATOM | 2251 | CA | GLY | B | 30 | 58.486 | 27.104 | 4.259 | 1.00 | 28.75 | C |
| ATOM | 2252 | C | GLY | B | 30 | 57.729 | 27.901 | 3.218 | 1.00 | 28.55 | C |
| ATOM | 2253 | O | GLY | B | 30 | 56.986 | 28.836 | 3.533 | 1.00 | 28.42 | O |
| ATOM | 2254 | N | THR | B | 31 | 57.942 | 27.515 | 1.963 | 1.00 | 28.38 | N |
| ATOM | 2255 | CA | THR | B | 31 | 57.261 | 28.101 | 0.818 | 1.00 | 28.05 | C |
| ATOM | 2256 | C | THR | B | 31 | 56.234 | 27.102 | 0.302 | 1.00 | 28.03 | C |
| ATOM | 2257 | O | THR | B | 31 | 56.569 | 25.958 | -0.013 | 1.00 | 28.03 | O |
| ATOM | 2258 | CB | THR | B | 31 | 58.281 | 28.454 | -0.285 | 1.00 | 27.97 | C |
| ATOM | 2259 | OG1 | THR | B | 31 | 59.191 | 29.447 | 0.205 | 1.00 | 27.82 | O |
| ATOM | 2260 | CG2 | THR | B | 31 | 57.601 | 29.149 | -1.460 | 1.00 | 27.96 | C |
| ATOM | 2261 | N | VAL | B | 32 | 54.982 | 27.540 | 0.228 | 1.00 | 27.96 | N |
| ATOM | 2262 | CA | VAL | B | 32 | 53.903 | 26.691 | -0.264 | 1.00 | 27.86 | C |
| ATOM | 2263 | C | VAL | B | 32 | 53.731 | 26.877 | -1.768 | 1.00 | 27.85 | C |
| ATOM | 2264 | O | VAL | B | 32 | 53.748 | 28.001 | -2.277 | 1.00 | 28.03 | O |
| ATOM | 2265 | CB | VAL | B | 32 | 52.575 | 26.939 | 0.495 | 1.00 | 27.79 | C |
| ATOM | 2266 | CG1 | VAL | B | 32 | 51.461 | 26.052 | -0.042 | 1.00 | 27.78 | C |
| ATOM | 2267 | CG2 | VAL | B | 32 | 52.762 | 26.679 | 1.982 | 1.00 | 27.76 | C |
| ATOM | 2268 | N | TYR | B | 33 | 53.583 | 25.758 | -2.469 | 1.00 | 27.72 | N |
| ATOM | 2269 | CA | TYR | B | 33 | 53.424 | 25.753 | -3.912 | 1.00 | 27.67 | C |
| ATOM | 2270 | C | TYR | B | 33 | 52.108 | 25.103 | -4.302 | 1.00 | 27.56 | C |
| ATOM | 2271 | O | TYR | B | 33 | 51.662 | 24.150 | -3.664 | 1.00 | 27.55 | O |
| ATOM | 2272 | CB | TYR | B | 33 | 54.566 | 24.975 | -4.575 | 1.00 | 27.76 | C |
| ATOM | 2273 | CG | TYR | B | 33 | 55.937 | 25.586 | -4.409 | 1.00 | 28.13 | C |
| ATOM | 2274 | CD1 | TYR | B | 33 | 56.438 | 26.487 | -5.349 | 1.00 | 28.14 | C |
| ATOM | 2275 | CE1 | TYR | B | 33 | 57.704 | 27.046 | -5.203 | 1.00 | 28.57 | C |

FIG. 4LL

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|---------|------|-------|---|
| ATOM | 2276 | CZ | TYR | B | 33 | 58.482 | 26.702 | -4.107 | 1.00 | 28.87 | C |
| ATOM | 2277 | OH | TYR | B | 33 | 59.733 | 27.254 | -3.954 | 1.00 | 29.32 | O |
| ATOM | 2278 | CE2 | TYR | B | 33 | 58.008 | 25.806 | -3.161 | 1.00 | 28.67 | C |
| ATOM | 2279 | CD2 | TYR | B | 33 | 56.742 | 25.252 | -3.317 | 1.00 | 28.47 | C |
| ATOM | 2280 | N | LYS | B | 34 | 51.490 | 25.636 | -5.351 | 1.00 | 27.51 | N |
| ATOM | 2281 | CA | LYS | B | 34 | 50.421 | 24.944 | -6.053 | 1.00 | 27.50 | C |
| ATOM | 2282 | C | LYS | B | 34 | 51.083 | 24.054 | -7.089 | 1.00 | 27.38 | C |
| ATOM | 2283 | O | LYS | B | 34 | 51.898 | 24.526 | -7.888 | 1.00 | 27.32 | O |
| ATOM | 2284 | CB | LYS | B | 34 | 49.486 | 25.942 | -6.734 | 1.00 | 27.57 | C |
| ATOM | 2285 | CG | LYS | B | 34 | 48.187 | 26.168 | -5.998 | 1.00 | 27.81 | C |
| ATOM | 2286 | CD | LYS | B | 34 | 47.135 | 26.770 | -6.904 | 1.00 | 28.47 | C |
| ATOM | 2287 | CE | LYS | B | 34 | 46.836 | 28.209 | -6.521 | 1.00 | 28.61 | C |
| ATOM | 2288 | NZ | LYS | B | 34 | 47.432 | 29.170 | -7.494 | 1.00 | 28.86 | N |
| ATOM | 2289 | N | GLY | B | 35 | 50.746 | 22.767 | -7.067 | 1.00 | 27.38 | N |
| ATOM | 2290 | CA | GLY | B | 35 | 51.364 | 21.805 | -7.964 | 1.00 | 27.34 | C |
| ATOM | 2291 | C | GLY | B | 35 | 50.546 | 20.565 | -8.257 | 1.00 | 27.34 | C |
| ATOM | 2292 | O | GLY | B | 35 | 49.432 | 20.406 | -7.757 | 1.00 | 26.97 | O |
| ATOM | 2293 | N | LEU | B | 36 | 51.116 | 19.685 | -9.075 | 1.00 | 27.72 | N |
| ATOM | 2294 | CA | LEU | B | 36 | 50.453 | 18.456 | -9.500 | 1.00 | 28.11 | C |
| ATOM | 2295 | C | LEU | B | 36 | 51.096 | 17.223 | -8.882 | 1.00 | 28.41 | C |
| ATOM | 2296 | O | LEU | B | 36 | 52.315 | 17.161 | -8.727 | 1.00 | 28.37 | O |
| ATOM | 2297 | CB | LEU | B | 36 | 50.482 | 18.332 | -11.026 | 1.00 | 28.07 | C |
| ATOM | 2298 | CG | LEU | B | 36 | 49.272 | 18.800 | -11.843 | 1.00 | 28.21 | C |
| ATOM | 2299 | CD1 | LEU | B | 36 | 49.582 | 18.707 | -13.327 | 1.00 | 28.16 | C |
| ATOM | 2300 | CD2 | LEU | B | 36 | 48.011 | 18.007 | -11.516 | 1.00 | 28.23 | C |
| ATOM | 2301 | N | TRP | B | 37 | 50.261 | 16.249 | -8.533 | 1.00 | 28.91 | N |
| ATOM | 2302 | CA | TRP | B | 37 | 50.717 | 14.964 | -8.018 | 1.00 | 29.48 | C |
| ATOM | 2303 | C | TRP | B | 37 | 50.344 | 13.868 | -9.010 | 1.00 | 29.70 | C |
| ATOM | 2304 | O | TRP | B | 37 | 49.168 | 13.680 | -9.326 | 1.00 | 29.69 | O |
| ATOM | 2305 | CB | TRP | B | 37 | 50.097 | 14.686 | -6.642 | 1.00 | 29.68 | C |
| ATOM | 2306 | CG | TRP | B | 37 | 50.548 | 13.401 | -5.978 | 1.00 | 30.20 | C |
| ATOM | 2307 | CD1 | TRP | B | 37 | 51.660 | 12.658 | -6.275 | 1.00 | 30.53 | C |
| ATOM | 2308 | NE1 | TRP | B | 37 | 51.731 | 11.558 | -5.454 | 1.00 | 30.58 | N |
| ATOM | 2309 | CE2 | TRP | B | 37 | 50.663 | 11.572 | -4.597 | 1.00 | 30.67 | C |
| ATOM | 2310 | CD2 | TRP | B | 37 | 49.896 | 12.720 | -4.899 | 1.00 | 30.54 | C |
| ATOM | 2311 | CE3 | TRP | B | 37 | 48.735 | 12.962 | -4.152 | 1.00 | 30.95 | C |
| ATOM | 2312 | CZ3 | TRP | B | 37 | 48.382 | 12.067 | -3.146 | 1.00 | 31.27 | C |
| ATOM | 2313 | CH2 | TRP | B | 37 | 49.168 | 10.937 | -2.874 | 1.00 | 31.31 | C |
| ATOM | 2314 | CZ2 | TRP | B | 37 | 50.308 | 10.673 | -3.586 | 1.00 | 31.05 | C |
| ATOM | 2315 | N | ILE | B | 38 | 51.356 | 13.158 | -9.502 | 1.00 | 30.12 | N |
| ATOM | 2316 | CA | ILE | B | 38 | 51.165 | 12.096 | -10.486 | 1.00 | 30.54 | C |
| ATOM | 2317 | C | ILE | B | 38 | 51.885 | 10.816 | -10.062 | 1.00 | 30.68 | C |
| ATOM | 2318 | O | ILE | B | 38 | 53.090 | 10.675 | -10.283 | 1.00 | 30.85 | O |
| ATOM | 2319 | CB | ILE | B | 38 | 51.641 | 12.553 | -11.888 | 1.00 | 30.47 | C |
| ATOM | 2320 | N | PRO | B | 39 | 51.145 | 9.888 | -9.454 | 1.00 | 31.01 | N |
| ATOM | 2321 | CA | PRO | B | 39 | 51.718 | 8.615 | -8.994 | 1.00 | 31.14 | C |
| ATOM | 2322 | C | PRO | B | 39 | 51.989 | 7.643 | -10.144 | 1.00 | 31.39 | C |
| ATOM | 2323 | O | PRO | B | 39 | 51.586 | 7.906 | -11.282 | 1.00 | 31.62 | O |
| ATOM | 2324 | CB | PRO | B | 39 | 50.629 | 8.058 | -8.075 | 1.00 | 31.16 | C |
| ATOM | 2325 | CG | PRO | B | 39 | 49.352 | 8.637 | -8.602 | 1.00 | 31.20 | C |
| ATOM | 2326 | CD | PRO | B | 39 | 49.701 | 9.986 | -9.162 | 1.00 | 31.03 | C |
| ATOM | 2327 | N | ILE | B | 46 | 46.081 | 15.307 | -10.527 | 1.00 | 24.43 | N |
| ATOM | 2328 | CA | ILE | B | 46 | 45.702 | 15.591 | -9.143 | 1.00 | 24.50 | C |
| ATOM | 2329 | C | ILE | B | 46 | 46.391 | 16.852 | -8.602 | 1.00 | 24.43 | C |
| ATOM | 2330 | O | ILE | B | 46 | 47.552 | 16.799 | -8.192 | 1.00 | 24.34 | O |
| ATOM | 2331 | CB | ILE | B | 46 | 45.997 | 14.375 | -8.233 | 1.00 | 24.30 | C |
| ATOM | 2332 | N | PRO | B | 47 | 45.680 | 17.982 | -8.617 | 1.00 | 24.47 | N |
| ATOM | 2333 | CA | PRO | B | 47 | 46.200 | 19.240 | -8.061 | 1.00 | 24.46 | C |
| ATOM | 2334 | C | PRO | B | 47 | 46.413 | 19.134 | -6.554 | 1.00 | 24.35 | C |
| ATOM | 2335 | O | PRO | B | 47 | 45.622 | 18.488 | -5.863 | 1.00 | 24.56 | O |

FIG. 4MM

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2336 | CB | PRO | B | 47 | 45.092 | 20.249 | -8.379 | 1.00 | 24.56 | C |
| ATOM | 2337 | CG | PRO | B | 47 | 44.313 | 19.618 | -9.487 | 1.00 | 24.65 | C |
| ATOM | 2338 | CD | PRO | B | 47 | 44.328 | 18.152 | -9.181 | 1.00 | 24.51 | C |
| ATOM | 2339 | N | VAL | B | 48 | 47.469 | 19.772 | -6.056 | 1.00 | 24.13 | N |
| ATOM | 2340 | CA | VAL | B | 48 | 47.947 | 19.531 | -4.700 | 1.00 | 23.96 | C |
| ATOM | 2341 | C | VAL | B | 48 | 48.742 | 20.722 | -4.148 | 1.00 | 24.14 | C |
| ATOM | 2342 | O | VAL | B | 48 | 49.158 | 21.606 | -4.904 | 1.00 | 24.29 | O |
| ATOM | 2343 | CB | VAL | B | 48 | 48.780 | 18.204 | -4.661 | 1.00 | 23.97 | C |
| ATOM | 2344 | CG1 | VAL | B | 48 | 50.295 | 18.459 | -4.708 | 1.00 | 23.50 | C |
| ATOM | 2345 | CG2 | VAL | B | 48 | 48.376 | 17.345 | -3.481 | 1.00 | 23.89 | C |
| ATOM | 2346 | N | ALA | B | 49 | 48.933 | 20.754 | -2.831 | 1.00 | 24.09 | N |
| ATOM | 2347 | CA | ALA | B | 49 | 49.784 | 21.761 | -2.203 | 1.00 | 24.09 | C |
| ATOM | 2348 | C | ALA | B | 49 | 51.132 | 21.155 | -1.821 | 1.00 | 24.22 | C |
| ATOM | 2349 | O | ALA | B | 49 | 51.187 | 20.081 | -1.224 | 1.00 | 24.15 | O |
| ATOM | 2350 | CB | ALA | B | 49 | 49.098 | 22.357 | -0.982 | 1.00 | 23.99 | C |
| ATOM | 2351 | N | ILE | B | 50 | 52.214 | 21.843 | -2.180 | 1.00 | 24.48 | N |
| ATOM | 2352 | CA | ILE | B | 50 | 53.566 | 21.409 | -1.828 | 1.00 | 24.74 | C |
| ATOM | 2353 | C | ILE | B | 50 | 54.239 | 22.459 | -0.952 | 1.00 | 24.99 | C |
| ATOM | 2354 | O | ILE | B | 50 | 54.338 | 23.620 | -1.334 | 1.00 | 25.01 | O |
| ATOM | 2355 | CB | ILE | B | 50 | 54.425 | 21.126 | -3.094 | 1.00 | 24.73 | C |
| ATOM | 2356 | CG1 | ILE | B | 50 | 53.696 | 20.184 | -4.056 | 1.00 | 24.79 | C |
| ATOM | 2357 | CD1 | ILE | B | 50 | 53.807 | 20.587 | -5.505 | 1.00 | 24.50 | C |
| ATOM | 2358 | CG2 | ILE | B | 50 | 55.780 | 20.530 | -2.712 | 1.00 | 24.47 | C |
| ATOM | 2359 | N | LYS | B | 51 | 54.691 | 22.043 | 0.227 | 1.00 | 25.49 | N |
| ATOM | 2360 | CA | LYS | B | 51 | 55.411 | 22.928 | 1.134 | 1.00 | 25.82 | C |
| ATOM | 2361 | C | LYS | B | 51 | 56.863 | 22.481 | 1.271 | 1.00 | 26.19 | C |
| ATOM | 2362 | O | LYS | B | 51 | 57.149 | 21.360 | 1.697 | 1.00 | 26.02 | O |
| ATOM | 2363 | CB | LYS | B | 51 | 54.729 | 22.981 | 2.502 | 1.00 | 25.80 | C |
| ATOM | 2364 | N | GLU | B | 52 | 57.773 | 23.373 | 0.896 | 1.00 | 26.64 | N |
| ATOM | 2365 | CA | GLU | B | 52 | 59.199 | 23.096 | 0.940 | 1.00 | 27.12 | C |
| ATOM | 2366 | C | GLU | B | 52 | 59.835 | 23.899 | 2.065 | 1.00 | 27.24 | C |
| ATOM | 2367 | O | GLU | B | 52 | 59.854 | 25.134 | 2.023 | 1.00 | 27.28 | O |
| ATOM | 2368 | CB | GLU | B | 52 | 59.836 | 23.448 | -0.405 | 1.00 | 27.40 | C |
| ATOM | 2369 | CG | GLU | B | 52 | 61.252 | 22.931 | -0.593 | 1.00 | 28.38 | C |
| ATOM | 2370 | CD | GLU | B | 52 | 61.769 | 23.156 | -1.999 | 1.00 | 29.42 | C |
| ATOM | 2371 | OE1 | GLU | B | 52 | 61.627 | 24.287 | -2.522 | 1.00 | 29.75 | O |
| ATOM | 2372 | OE2 | GLU | B | 52 | 62.317 | 22.197 | -2.583 | 1.00 | 30.05 | O |
| ATOM | 2373 | N | LEU | B | 53 | 60.348 | 23.191 | 3.069 | 1.00 | 27.29 | N |
| ATOM | 2374 | CA | LEU | B | 53 | 60.956 | 23.824 | 4.238 | 1.00 | 27.37 | C |
| ATOM | 2375 | C | LEU | B | 53 | 62.152 | 24.688 | 3.850 | 1.00 | 27.87 | C |
| ATOM | 2376 | O | LEU | B | 53 | 62.920 | 24.335 | 2.952 | 1.00 | 28.04 | O |
| ATOM | 2377 | CB | LEU | B | 53 | 61.373 | 22.773 | 5.274 | 1.00 | 27.04 | C |
| ATOM | 2378 | CG | LEU | B | 53 | 60.352 | 21.766 | 5.832 | 1.00 | 26.54 | C |
| ATOM | 2379 | CD1 | LEU | B | 53 | 60.925 | 21.073 | 7.065 | 1.00 | 26.17 | C |
| ATOM | 2380 | CD2 | LEU | B | 53 | 58.997 | 22.395 | 6.161 | 1.00 | 25.66 | C |
| ATOM | 2381 | N | ARG | B | 54 | 62.297 | 25.823 | 4.531 | 1.00 | 28.51 | N |
| ATOM | 2382 | CA | ARG | B | 54 | 63.370 | 26.782 | 4.249 | 1.00 | 29.00 | C |
| ATOM | 2383 | C | ARG | B | 54 | 64.755 | 26.212 | 4.539 | 1.00 | 28.95 | C |
| ATOM | 2384 | O | ARG | B | 54 | 65.747 | 26.653 | 3.951 | 1.00 | 29.33 | O |
| ATOM | 2385 | CB | ARG | B | 54 | 63.163 | 28.090 | 5.025 | 1.00 | 29.38 | C |
| ATOM | 2386 | CG | ARG | B | 54 | 62.529 | 27.924 | 6.401 | 1.00 | 30.65 | C |
| ATOM | 2387 | CD | ARG | B | 54 | 63.325 | 28.546 | 7.534 | 1.00 | 32.35 | C |
| ATOM | 2388 | NE | ARG | B | 54 | 62.677 | 29.745 | 8.061 | 1.00 | 33.88 | N |
| ATOM | 2389 | CZ | ARG | B | 54 | 62.675 | 30.103 | 9.342 | 1.00 | 34.80 | C |
| ATOM | 2390 | NH1 | ARG | B | 54 | 62.053 | 31.216 | 9.715 | 1.00 | 35.20 | N |
| ATOM | 2391 | NH2 | ARG | B | 54 | 63.282 | 29.352 | 10.255 | 1.00 | 35.03 | N |
| ATOM | 2392 | N | GLU | B | 55 | 64.817 | 25.239 | 5.446 | 1.00 | 28.69 | N |
| ATOM | 2393 | CA | GLU | B | 55 | 66.070 | 24.560 | 5.768 | 1.00 | 28.61 | C |
| ATOM | 2394 | C | GLU | B | 55 | 66.053 | 23.114 | 5.279 | 1.00 | 28.60 | C |
| ATOM | 2395 | O | GLU | B | 55 | 65.046 | 22.632 | 4.757 | 1.00 | 28.57 | O |

FIG. 4NN

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2396 | CB | GLU | B | 55 | 66.336 | 24.604 | 7.274 | 1.00 | 28.56 | C |
| ATOM | 2397 | N | LYS | B | 63 | 65.778 | 10.560 | 9.002 | 1.00 | 30.12 | N |
| ATOM | 2398 | CA | LYS | B | 63 | 65.123 | 9.381 | 9.558 | 1.00 | 30.00 | C |
| ATOM | 2399 | C | LYS | B | 63 | 63.989 | 9.762 | 10.509 | 1.00 | 30.00 | C |
| ATOM | 2400 | O | LYS | B | 63 | 62.857 | 9.301 | 10.348 | 1.00 | 30.03 | O |
| ATOM | 2401 | CB | LYS | B | 63 | 66.140 | 8.487 | 10.272 | 1.00 | 29.90 | C |
| ATOM | 2402 | N | GLU | B | 64 | 64.302 | 10.604 | 11.493 | 1.00 | 30.01 | N |
| ATOM | 2403 | CA | GLU | B | 64 | 63.332 | 11.037 | 12.500 | 1.00 | 29.98 | C |
| ATOM | 2404 | C | GLU | B | 64 | 62.302 | 12.005 | 11.917 | 1.00 | 29.81 | C |
| ATOM | 2405 | O | GLU | B | 64 | 61.177 | 12.096 | 12.414 | 1.00 | 29.67 | O |
| ATOM | 2406 | CB | GLU | B | 64 | 64.044 | 11.672 | 13.698 | 1.00 | 30.05 | C |
| ATOM | 2407 | N | ILE | B | 65 | 62.703 | 12.722 | 10.868 | 1.00 | 29.64 | N |
| ATOM | 2408 | CA | ILE | B | 65 | 61.807 | 13.593 | 10.106 | 1.00 | 29.46 | C |
| ATOM | 2409 | C | ILE | B | 65 | 60.683 | 12.774 | 9.462 | 1.00 | 29.27 | C |
| ATOM | 2410 | O | ILE | B | 65 | 59.520 | 13.187 | 9.475 | 1.00 | 29.16 | O |
| ATOM | 2411 | CB | ILE | B | 65 | 62.594 | 14.374 | 9.022 | 1.00 | 29.61 | C |
| ATOM | 2412 | CG1 | ILE | B | 65 | 63.901 | 14.934 | 9.592 | 1.00 | 29.86 | C |
| ATOM | 2413 | CD1 | ILE | B | 65 | 65.146 | 14.350 | 8.953 | 1.00 | 30.24 | C |
| ATOM | 2414 | CG2 | ILE | B | 65 | 61.747 | 15.503 | 8.440 | 1.00 | 29.75 | C |
| ATOM | 2415 | N | LEU | B | 66 | 61.048 | 11.616 | 8.907 | 1.00 | 28.93 | N |
| ATOM | 2416 | CA | LEU | B | 66 | 60.096 | 10.680 | 8.312 | 1.00 | 28.66 | C |
| ATOM | 2417 | C | LEU | B | 66 | 59.178 | 10.072 | 9.371 | 1.00 | 28.51 | C |
| ATOM | 2418 | O | LEU | B | 66 | 57.992 | 9.856 | 9.118 | 1.00 | 28.64 | O |
| ATOM | 2419 | CB | LEU | B | 66 | 60.834 | 9.574 | 7.549 | 1.00 | 28.74 | C |
| ATOM | 2420 | CG | LEU | B | 66 | 60.010 | 8.543 | 6.769 | 1.00 | 28.85 | C |
| ATOM | 2421 | CD1 | LEU | B | 66 | 60.105 | 8.787 | 5.274 | 1.00 | 29.23 | C |
| ATOM | 2422 | CD2 | LEU | B | 66 | 60.469 | 7.134 | 7.102 | 1.00 | 29.04 | C |
| ATOM | 2423 | N | ASP | B | 67 | 59.730 | 9.803 | 10.553 | 1.00 | 28.24 | N |
| ATOM | 2424 | CA | ASP | B | 67 | 58.951 | 9.261 | 11.665 | 1.00 | 27.91 | C |
| ATOM | 2425 | C | ASP | B | 67 | 57.893 | 10.255 | 12.134 | 1.00 | 27.44 | C |
| ATOM | 2426 | O | ASP | B | 67 | 56.780 | 9.862 | 12.489 | 1.00 | 27.47 | O |
| ATOM | 2427 | CB | ASP | B | 67 | 59.861 | 8.860 | 12.826 | 1.00 | 28.21 | C |
| ATOM | 2428 | CG | ASP | B | 67 | 60.162 | 7.372 | 12.846 | 1.00 | 29.13 | C |
| ATOM | 2429 | OD1 | ASP | B | 67 | 61.339 | 7.010 | 13.066 | 1.00 | 30.16 | O |
| ATOM | 2430 | OD2 | ASP | B | 67 | 59.295 | 6.488 | 12.658 | 1.00 | 29.78 | O |
| ATOM | 2431 | N | GLU | B | 68 | 58.249 | 11.539 | 12.120 | 1.00 | 26.75 | N |
| ATOM | 2432 | CA | GLU | B | 68 | 57.320 | 12.617 | 12.446 | 1.00 | 26.21 | C |
| ATOM | 2433 | C | GLU | B | 68 | 56.264 | 12.790 | 11.355 | 1.00 | 25.93 | C |
| ATOM | 2434 | O | GLU | B | 68 | 55.138 | 13.210 | 11.632 | 1.00 | 25.86 | O |
| ATOM | 2435 | CB | GLU | B | 68 | 58.076 | 13.930 | 12.659 | 1.00 | 26.13 | C |
| ATOM | 2436 | N | ALA | B | 69 | 56.634 | 12.464 | 10.119 | 1.00 | 25.37 | N |
| ATOM | 2437 | CA | ALA | B | 69 | 55.713 | 12.540 | 8.988 | 1.00 | 24.87 | C |
| ATOM | 2438 | C | ALA | B | 69 | 54.645 | 11.448 | 9.049 | 1.00 | 24.63 | C |
| ATOM | 2439 | O | ALA | B | 69 | 53.526 | 11.644 | 8.566 | 1.00 | 24.51 | O |
| ATOM | 2440 | CB | ALA | B | 69 | 56.472 | 12.470 | 7.678 | 1.00 | 24.81 | C |
| ATOM | 2441 | N | TYR | B | 70 | 54.994 | 10.311 | 9.650 | 1.00 | 24.18 | N |
| ATOM | 2442 | CA | TYR | B | 70 | 54.066 | 9.190 | 9.799 | 1.00 | 23.84 | C |
| ATOM | 2443 | C | TYR | B | 70 | 52.915 | 9.508 | 10.753 | 1.00 | 23.49 | C |
| ATOM | 2444 | O | TYR | B | 70 | 51.761 | 9.188 | 10.456 | 1.00 | 23.32 | O |
| ATOM | 2445 | CB | TYR | B | 70 | 54.799 | 7.915 | 10.237 | 1.00 | 23.91 | C |
| ATOM | 2446 | CG | TYR | B | 70 | 55.306 | 7.080 | 9.080 | 1.00 | 23.87 | C |
| ATOM | 2447 | CD1 | TYR | B | 70 | 54.422 | 6.410 | 8.234 | 1.00 | 23.97 | C |
| ATOM | 2448 | CE1 | TYR | B | 70 | 54.887 | 5.648 | 7.162 | 1.00 | 23.97 | C |
| ATOM | 2449 | CZ | TYR | B | 70 | 56.250 | 5.551 | 6.935 | 1.00 | 23.96 | C |
| ATOM | 2450 | OH | TYR | B | 70 | 56.721 | 4.799 | 5.884 | 1.00 | 24.29 | O |
| ATOM | 2451 | CE2 | TYR | B | 70 | 57.145 | 6.206 | 7.761 | 1.00 | 23.92 | C |
| ATOM | 2452 | CD2 | TYR | B | 70 | 56.671 | 6.966 | 8.826 | 1.00 | 24.06 | C |
| ATOM | 2453 | N | VAL | B | 71 | 53.230 | 10.138 | 11.886 | 1.00 | 23.05 | N |
| ATOM | 2454 | CA | VAL | B | 71 | 52.200 | 10.587 | 12.827 | 1.00 | 22.77 | C |
| ATOM | 2455 | C | VAL | B | 71 | 51.390 | 11.739 | 12.224 | 1.00 | 22.40 | C |

FIG. 400

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2456 | O | VAL | B | 71 | 50.174 | 11.822 | 12.422 | 1.00 | 22.62 | O |
| ATOM | 2457 | CB | VAL | B | 71 | 52.772 | 10.931 | 14.250 | 1.00 | 22.74 | C |
| ATOM | 2458 | CG1 | VAL | B | 71 | 53.773 | 12.070 | 14.207 | 1.00 | 23.13 | C |
| ATOM | 2459 | CG2 | VAL | B | 71 | 51.651 | 11.249 | 15.235 | 1.00 | 22.86 | C |
| ATOM | 2460 | N | MET | B | 72 | 52.069 | 12.600 | 11.467 | 1.00 | 21.88 | N |
| ATOM | 2461 | CA | MET | B | 72 | 51.422 | 13.685 | 10.736 | 1.00 | 21.55 | C |
| ATOM | 2462 | C | MET | B | 72 | 50.433 | 13.158 | 9.699 | 1.00 | 21.36 | C |
| ATOM | 2463 | O | MET | B | 72 | 49.385 | 13.762 | 9.472 | 1.00 | 21.11 | O |
| ATOM | 2464 | CB | MET | B | 72 | 52.467 | 14.565 | 10.052 | 1.00 | 21.63 | C |
| ATOM | 2465 | CG | MET | B | 72 | 52.969 | 15.709 | 10.910 | 1.00 | 21.62 | C |
| ATOM | 2466 | SD | MET | B | 72 | 54.562 | 16.324 | 10.351 | 1.00 | 22.13 | S |
| ATOM | 2467 | CE | MET | B | 72 | 54.058 | 17.466 | 9.116 | 1.00 | 21.51 | C |
| ATOM | 2468 | N | ALA | B | 73 | 50.774 | 12.026 | 9.083 | 1.00 | 21.09 | N |
| ATOM | 2469 | CA | ALA | B | 73 | 49.915 | 11.378 | 8.095 | 1.00 | 20.63 | C |
| ATOM | 2470 | C | ALA | B | 73 | 48.847 | 10.486 | 8.722 | 1.00 | 20.41 | C |
| ATOM | 2471 | O | ALA | B | 73 | 47.914 | 10.059 | 8.038 | 1.00 | 20.42 | O |
| ATOM | 2472 | CB | ALA | B | 73 | 50.749 | 10.582 | 7.123 | 1.00 | 20.70 | C |
| ATOM | 2473 | N | SER | B | 74 | 48.989 | 10.196 | 10.014 | 1.00 | 20.08 | N |
| ATOM | 2474 | CA | SER | B | 74 | 48.030 | 9.345 | 10.716 | 1.00 | 19.66 | C |
| ATOM | 2475 | C | SER | B | 74 | 46.854 | 10.157 | 11.247 | 1.00 | 19.50 | C |
| ATOM | 2476 | O | SER | B | 74 | 45.828 | 9.593 | 11.645 | 1.00 | 19.48 | O |
| ATOM | 2477 | CB | SER | B | 74 | 48.709 | 8.562 | 11.849 | 1.00 | 19.56 | C |
| ATOM | 2478 | OG | SER | B | 74 | 48.996 | 9.388 | 12.964 | 1.00 | 19.37 | O |
| ATOM | 2479 | N | VAL | B | 75 | 47.017 | 11.480 | 11.248 | 1.00 | 19.07 | N |
| ATOM | 2480 | CA | VAL | B | 75 | 45.996 | 12.404 | 11.735 | 1.00 | 18.77 | C |
| ATOM | 2481 | C | VAL | B | 75 | 44.693 | 12.257 | 10.951 | 1.00 | 18.64 | C |
| ATOM | 2482 | O | VAL | B | 75 | 44.611 | 12.595 | 9.770 | 1.00 | 18.83 | O |
| ATOM | 2483 | CB | VAL | B | 75 | 46.501 | 13.872 | 11.719 | 1.00 | 18.82 | C |
| ATOM | 2484 | CG1 | VAL | B | 75 | 45.350 | 14.854 | 11.885 | 1.00 | 18.76 | C |
| ATOM | 2485 | CG2 | VAL | B | 75 | 47.535 | 14.084 | 12.815 | 1.00 | 18.78 | C |
| ATOM | 2486 | N | ASP | B | 76 | 43.682 | 11.729 | 11.628 | 1.00 | 18.53 | N |
| ATOM | 2487 | CA | ASP | B | 76 | 42.377 | 11.516 | 11.024 | 1.00 | 18.29 | C |
| ATOM | 2488 | C | ASP | B | 76 | 41.298 | 12.265 | 11.807 | 1.00 | 17.84 | C |
| ATOM | 2489 | O | ASP | B | 76 | 40.775 | 11.763 | 12.805 | 1.00 | 17.73 | O |
| ATOM | 2490 | CB | ASP | B | 76 | 42.073 | 10.018 | 10.946 | 1.00 | 18.50 | C |
| ATOM | 2491 | CG | ASP | B | 76 | 40.947 | 9.698 | 9.987 | 1.00 | 19.04 | C |
| ATOM | 2492 | OD1 | ASP | B | 76 | 40.583 | 10.569 | 9.167 | 1.00 | 19.61 | O |
| ATOM | 2493 | OD2 | ASP | B | 76 | 40.364 | 8.593 | 9.981 | 1.00 | 19.97 | O |
| ATOM | 2494 | N | ASN | B | 77 | 40.993 | 13.477 | 11.347 | 1.00 | 17.35 | N |
| ATOM | 2495 | CA | ASN | B | 77 | 39.979 | 14.337 | 11.952 | 1.00 | 17.09 | C |
| ATOM | 2496 | C | ASN | B | 77 | 39.427 | 15.327 | 10.924 | 1.00 | 16.97 | C |
| ATOM | 2497 | O | ASN | B | 77 | 40.200 | 15.938 | 10.183 | 1.00 | 16.85 | O |
| ATOM | 2498 | CB | ASN | B | 77 | 40.554 | 15.092 | 13.157 | 1.00 | 17.00 | C |
| ATOM | 2499 | CG | ASN | B | 77 | 39.495 | 15.860 | 13.929 | 1.00 | 16.91 | C |
| ATOM | 2500 | OD1 | ASN | B | 77 | 39.183 | 17.007 | 13.609 | 1.00 | 16.63 | O |
| ATOM | 2501 | ND2 | ASN | B | 77 | 38.933 | 15.226 | 14.951 | 1.00 | 17.35 | N |
| ATOM | 2502 | N | PRO | B | 78 | 38.100 | 15.482 | 10.880 | 1.00 | 16.91 | N |
| ATOM | 2503 | CA | PRO | B | 78 | 37.446 | 16.410 | 9.941 | 1.00 | 16.93 | C |
| ATOM | 2504 | C | PRO | B | 78 | 37.894 | 17.870 | 10.073 | 1.00 | 17.03 | C |
| ATOM | 2505 | O | PRO | B | 78 | 37.616 | 18.670 | 9.179 | 1.00 | 16.85 | O |
| ATOM | 2506 | CB | PRO | B | 78 | 35.960 | 16.292 | 10.308 | 1.00 | 16.95 | C |
| ATOM | 2507 | CG | PRO | B | 78 | 35.830 | 14.978 | 10.994 | 1.00 | 16.68 | C |
| ATOM | 2508 | CD | PRO | B | 78 | 37.118 | 14.759 | 11.710 | 1.00 | 16.84 | C |
| ATOM | 2509 | N | HIS | B | 79 | 38.576 | 18.208 | 11.164 | 1.00 | 17.24 | N |
| ATOM | 2510 | CA | HIS | B | 79 | 38.994 | 19.588 | 11.399 | 1.00 | 17.45 | C |
| ATOM | 2511 | C | HIS | B | 79 | 40.508 | 19.772 | 11.531 | 1.00 | 17.57 | C |
| ATOM | 2512 | O | HIS | B | 79 | 40.973 | 20.834 | 11.949 | 1.00 | 17.58 | O |
| ATOM | 2513 | CB | HIS | B | 79 | 38.246 | 20.172 | 12.602 | 1.00 | 17.43 | C |
| ATOM | 2514 | CG | HIS | B | 79 | 36.758 | 20.152 | 12.444 | 1.00 | 17.41 | C |
| ATOM | 2515 | ND1 | HIS | B | 79 | 36.112 | 20.784 | 11.404 | 1.00 | 17.41 | N |

FIG. 4PP

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2516 | CE1 | HIS | B | 79 | 34.811 | 20.587 | 11.511 | 1.00 | 17.51 | C |
| ATOM | 2517 | NE2 | HIS | B | 79 | 34.589 | 19.849 | 12.583 | 1.00 | 17.39 | N |
| ATOM | 2518 | CD2 | HIS | B | 79 | 35.791 | 19.559 | 13.182 | 1.00 | 17.34 | C |
| ATOM | 2519 | N | VAL | B | 80 | 41.268 | 18.736 | 11.175 | 1.00 | 17.71 | N |
| ATOM | 2520 | CA | VAL | B | 80 | 42.720 | 18.848 | 11.033 | 1.00 | 18.13 | C |
| ATOM | 2521 | C | VAL | B | 80 | 43.138 | 18.311 | 9.665 | 1.00 | 18.46 | C |
| ATOM | 2522 | O | VAL | B | 80 | 42.771 | 17.195 | 9.294 | 1.00 | 18.65 | O |
| ATOM | 2523 | CB | VAL | B | 80 | 43.510 | 18.100 | 12.148 | 1.00 | 18.16 | C |
| ATOM | 2524 | CG1 | VAL | B | 80 | 44.978 | 18.517 | 12.134 | 1.00 | 18.02 | C |
| ATOM | 2525 | CG2 | VAL | B | 80 | 42.911 | 18.343 | 13.528 | 1.00 | 17.79 | C |
| ATOM | 2526 | N | CYS | B | 81 | 43.893 | 19.114 | 8.920 | 1.00 | 18.84 | N |
| ATOM | 2527 | CA | CYS | B | 81 | 44.410 | 18.706 | 7.614 | 1.00 | 19.24 | C |
| ATOM | 2528 | C | CYS | B | 81 | 45.411 | 17.572 | 7.772 | 1.00 | 19.26 | C |
| ATOM | 2529 | O | CYS | B | 81 | 46.147 | 17.526 | 8.749 | 1.00 | 19.30 | O |
| ATOM | 2530 | CB | CYS | B | 81 | 45.066 | 19.884 | 6.898 | 1.00 | 19.33 | C |
| ATOM | 2531 | SG | CYS | B | 81 | 43.932 | 21.220 | 6.469 | 1.00 | 19.69 | S |
| ATOM | 2532 | N | ARG | B | 82 | 45.424 | 16.659 | 6.808 | 1.00 | 19.54 | N |
| ATOM | 2533 | CA | ARG | B | 82 | 46.262 | 15.467 | 6.867 | 1.00 | 19.86 | C |
| ATOM | 2534 | C | ARG | B | 82 | 47.445 | 15.591 | 5.912 | 1.00 | 20.02 | C |
| ATOM | 2535 | O | ARG | B | 82 | 47.330 | 16.198 | 4.845 | 1.00 | 20.28 | O |
| ATOM | 2536 | CB | ARG | B | 82 | 45.421 | 14.235 | 6.511 | 1.00 | 19.91 | C |
| ATOM | 2537 | CG | ARG | B | 82 | 46.039 | 12.888 | 6.854 | 1.00 | 20.11 | C |
| ATOM | 2538 | CD | ARG | B | 82 | 45.336 | 11.707 | 6.184 | 1.00 | 20.60 | C |
| ATOM | 2539 | NE | ARG | B | 82 | 46.261 | 10.623 | 5.854 | 1.00 | 20.98 | N |
| ATOM | 2540 | CZ | ARG | B | 82 | 46.402 | 10.082 | 4.647 | 1.00 | 21.13 | C |
| ATOM | 2541 | NH1 | ARG | B | 82 | 45.682 | 10.511 | 3.620 | 1.00 | 21.34 | N |
| ATOM | 2542 | NH2 | ARG | B | 82 | 47.273 | 9.103 | 4.464 | 1.00 | 21.49 | N |
| ATOM | 2543 | N | LEU | B | 83 | 48.583 | 15.026 | 6.306 | 1.00 | 20.21 | N |
| ATOM | 2544 | CA | LEU | B | 83 | 49.722 | 14.902 | 5.404 | 1.00 | 20.33 | C |
| ATOM | 2545 | C | LEU | B | 83 | 49.494 | 13.715 | 4.478 | 1.00 | 20.42 | C |
| ATOM | 2546 | O | LEU | B | 83 | 49.357 | 12.577 | 4.935 | 1.00 | 20.56 | O |
| ATOM | 2547 | CB | LEU | B | 83 | 51.035 | 14.741 | 6.179 | 1.00 | 20.20 | C |
| ATOM | 2548 | CG | LEU | B | 83 | 52.332 | 14.813 | 5.359 | 1.00 | 20.36 | C |
| ATOM | 2549 | CD1 | LEU | B | 83 | 52.515 | 16.180 | 4.702 | 1.00 | 20.37 | C |
| ATOM | 2550 | CD2 | LEU | B | 83 | 53.536 | 14.473 | 6.219 | 1.00 | 20.49 | C |
| ATOM | 2551 | N | LEU | B | 84 | 49.434 | 13.991 | 3.179 | 1.00 | 20.41 | N |
| ATOM | 2552 | CA | LEU | B | 84 | 49.234 | 12.946 | 2.182 | 1.00 | 20.44 | C |
| ATOM | 2553 | C | LEU | B | 84 | 50.548 | 12.244 | 1.851 | 1.00 | 20.54 | C |
| ATOM | 2554 | O | LEU | B | 84 | 50.575 | 11.024 | 1.682 | 1.00 | 20.69 | O |
| ATOM | 2555 | CB | LEU | B | 84 | 48.587 | 13.507 | 0.908 | 1.00 | 20.45 | C |
| ATOM | 2556 | CG | LEU | B | 84 | 47.294 | 14.333 | 0.997 | 1.00 | 20.58 | C |
| ATOM | 2557 | CD1 | LEU | B | 84 | 46.972 | 14.930 | -0.360 | 1.00 | 20.93 | C |
| ATOM | 2558 | CD2 | LEU | B | 84 | 46.108 | 13.520 | 1.511 | 1.00 | 20.23 | C |
| ATOM | 2559 | N | GLY | B | 85 | 51.633 | 13.013 | 1.766 | 1.00 | 20.51 | N |
| ATOM | 2560 | CA | GLY | B | 85 | 52.925 | 12.463 | 1.398 | 1.00 | 20.68 | C |
| ATOM | 2561 | C | GLY | B | 85 | 54.140 | 13.314 | 1.727 | 1.00 | 20.81 | C |
| ATOM | 2562 | O | GLY | B | 85 | 54.017 | 14.456 | 2.175 | 1.00 | 20.72 | O |
| ATOM | 2563 | N | ILE | B | 86 | 55.319 | 12.741 | 1.493 | 1.00 | 20.93 | N |
| ATOM | 2564 | CA | ILE | B | 86 | 56.593 | 13.412 | 1.751 | 1.00 | 21.14 | C |
| ATOM | 2565 | C | ILE | B | 86 | 57.639 | 13.056 | 0.687 | 1.00 | 21.56 | C |
| ATOM | 2566 | O | ILE | B | 86 | 57.555 | 12.007 | 0.044 | 1.00 | 21.49 | O |
| ATOM | 2567 | CB | ILE | B | 86 | 57.107 | 13.090 | 3.196 | 1.00 | 21.03 | C |
| ATOM | 2568 | CG1 | ILE | B | 86 | 58.210 | 14.068 | 3.612 | 1.00 | 20.91 | C |
| ATOM | 2569 | CD1 | ILE | B | 86 | 58.426 | 14.175 | 5.105 | 1.00 | 21.16 | C |
| ATOM | 2570 | CG2 | ILE | B | 86 | 57.568 | 11.624 | 3.322 | 1.00 | 20.69 | C |
| ATOM | 2571 | N | CYS | B | 87 | 58.606 | 13.951 | 0.494 | 1.00 | 22.26 | N |
| ATOM | 2572 | CA | CYS | B | 87 | 59.760 | 13.684 | -0.360 | 1.00 | 22.87 | C |
| ATOM | 2573 | C | CYS | B | 87 | 61.014 | 14.298 | 0.248 | 1.00 | 23.09 | C |
| ATOM | 2574 | O | CYS | B | 87 | 61.115 | 15.519 | 0.387 | 1.00 | 23.42 | O |
| ATOM | 2575 | CB | CYS | B | 87 | 59.536 | 14.221 | -1.772 | 1.00 | 22.92 | C |

FIG. 4QQ

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2576 | SG | CYS | B | 87 | 60.881 | 13.836 | -2.922 | 1.00 | 24.10 | S |
| ATOM | 2577 | N | LEU | B | 88 | 61.964 | 13.440 | 0.607 | 1.00 | 23.42 | N |
| ATOM | 2578 | CA | LEU | B | 88 | 63.201 | 13.871 | 1.254 | 1.00 | 23.82 | C |
| ATOM | 2579 | C | LEU | B | 88 | 64.388 | 13.802 | 0.298 | 1.00 | 23.93 | C |
| ATOM | 2580 | O | LEU | B | 88 | 64.498 | 12.869 | -0.498 | 1.00 | 24.28 | O |
| ATOM | 2581 | CB | LEU | B | 88 | 63.476 | 13.022 | 2.498 | 1.00 | 23.75 | C |
| ATOM | 2582 | CG | LEU | B | 88 | 62.455 | 13.123 | 3.631 | 1.00 | 23.54 | C |
| ATOM | 2583 | CD1 | LEU | B | 88 | 62.037 | 11.736 | 4.082 | 1.00 | 23.49 | C |
| ATOM | 2584 | CD2 | LEU | B | 88 | 63.018 | 13.923 | 4.794 | 1.00 | 23.51 | C |
| ATOM | 2585 | N | VAL | B | 92 | 63.403 | 18.650 | 2.176 | 1.00 | 22.16 | N |
| ATOM | 2586 | CA | VAL | B | 92 | 62.142 | 18.200 | 2.760 | 1.00 | 22.16 | C |
| ATOM | 2587 | C | VAL | B | 92 | 60.972 | 18.893 | 2.068 | 1.00 | 21.94 | C |
| ATOM | 2588 | O | VAL | B | 92 | 60.873 | 20.122 | 2.074 | 1.00 | 21.95 | O |
| ATOM | 2589 | CB | VAL | B | 92 | 62.081 | 18.453 | 4.293 | 1.00 | 22.29 | C |
| ATOM | 2590 | CG1 | VAL | B | 92 | 61.048 | 17.549 | 4.952 | 1.00 | 22.26 | C |
| ATOM | 2591 | CG2 | VAL | B | 92 | 63.447 | 18.242 | 4.934 | 1.00 | 22.88 | C |
| ATOM | 2592 | N | GLN | B | 93 | 60.096 | 18.093 | 1.464 | 1.00 | 21.75 | N |
| ATOM | 2593 | CA | GLN | B | 93 | 58.944 | 18.608 | 0.731 | 1.00 | 21.48 | C |
| ATOM | 2594 | C | GLN | B | 93 | 57.666 | 17.910 | 1.178 | 1.00 | 21.26 | C |
| ATOM | 2595 | O | GLN | B | 93 | 57.556 | 16.684 | 1.104 | 1.00 | 21.27 | O |
| ATOM | 2596 | CB | GLN | B | 93 | 59.149 | 18.446 | -0.778 | 1.00 | 21.61 | C |
| ATOM | 2597 | CG | GLN | B | 93 | 60.103 | 19.464 | -1.384 | 1.00 | 21.92 | C |
| ATOM | 2598 | CD | GLN | B | 93 | 60.099 | 19.444 | -2.897 | 1.00 | 22.34 | C |
| ATOM | 2599 | OE1 | GLN | B | 93 | 59.216 | 20.029 | -3.528 | 1.00 | 22.32 | O |
| ATOM | 2600 | NE2 | GLN | B | 93 | 61.085 | 18.772 | -3.485 | 1.00 | 22.27 | N |
| ATOM | 2601 | N | LEU | B | 94 | 56.707 | 18.702 | 1.646 | 1.00 | 21.02 | N |
| ATOM | 2602 | CA | LEU | B | 94 | 55.459 | 18.174 | 2.189 | 1.00 | 20.82 | C |
| ATOM | 2603 | C | LEU | B | 94 | 54.289 | 18.444 | 1.251 | 1.00 | 20.71 | C |
| ATOM | 2604 | O | LEU | B | 94 | 54.091 | 19.571 | 0.797 | 1.00 | 20.41 | O |
| ATOM | 2605 | CB | LEU | B | 94 | 55.180 | 18.754 | 3.579 | 1.00 | 20.74 | C |
| ATOM | 2606 | CG | LEU | B | 94 | 56.273 | 18.565 | 4.637 | 1.00 | 20.89 | C |
| ATOM | 2607 | CD1 | LEU | B | 94 | 56.307 | 19.752 | 5.579 | 1.00 | 20.79 | C |
| ATOM | 2608 | CD2 | LEU | B | 94 | 56.098 | 17.262 | 5.407 | 1.00 | 20.65 | C |
| ATOM | 2609 | N | ILE | B | 95 | 53.525 | 17.395 | 0.966 | 1.00 | 20.61 | N |
| ATOM | 2610 | CA | ILE | B | 95 | 52.394 | 17.482 | 0.050 | 1.00 | 20.57 | C |
| ATOM | 2611 | C | ILE | B | 95 | 51.074 | 17.203 | 0.769 | 1.00 | 20.45 | C |
| ATOM | 2612 | O | ILE | B | 95 | 50.903 | 16.161 | 1.408 | 1.00 | 20.36 | O |
| ATOM | 2613 | CB | ILE | B | 95 | 52.604 | 16.568 | -1.202 | 1.00 | 20.61 | C |
| ATOM | 2614 | CG1 | ILE | B | 95 | 51.279 | 16.005 | -1.725 | 1.00 | 20.59 | C |
| ATOM | 2615 | CD1 | ILE | B | 95 | 51.385 | 15.339 | -3.074 | 1.00 | 21.15 | C |
| ATOM | 2616 | CG2 | ILE | B | 95 | 53.597 | 15.457 | -0.907 | 1.00 | 20.84 | C |
| ATOM | 2617 | N | THR | B | 96 | 50.158 | 18.163 | 0.671 | 1.00 | 20.38 | N |
| ATOM | 2618 | CA | THR | B | 96 | 48.836 | 18.063 | 1.283 | 1.00 | 20.31 | C |
| ATOM | 2619 | C | THR | B | 96 | 47.754 | 18.421 | 0.270 | 1.00 | 20.16 | C |
| ATOM | 2620 | O | THR | B | 96 | 48.052 | 18.866 | -0.839 | 1.00 | 19.97 | O |
| ATOM | 2621 | CB | THR | B | 96 | 48.724 | 18.993 | 2.517 | 1.00 | 20.47 | C |
| ATOM | 2622 | OG1 | THR | B | 96 | 49.302 | 20.272 | 2.219 | 1.00 | 20.71 | O |
| ATOM | 2623 | CG2 | THR | B | 96 | 49.565 | 18.470 | 3.682 | 1.00 | 20.47 | C |
| ATOM | 2624 | N | GLN | B | 97 | 46.498 | 18.222 | 0.658 | 1.00 | 20.23 | N |
| ATOM | 2625 | CA | GLN | B | 97 | 45.363 | 18.599 | -0.174 | 1.00 | 20.15 | C |
| ATOM | 2626 | C | GLN | B | 97 | 45.330 | 20.107 | -0.409 | 1.00 | 19.95 | C |
| ATOM | 2627 | O | GLN | B | 97 | 45.513 | 20.902 | 0.519 | 1.00 | 19.89 | O |
| ATOM | 2628 | CB | GLN | B | 97 | 44.054 | 18.139 | 0.464 | 1.00 | 20.26 | C |
| ATOM | 2629 | CG | GLN | B | 97 | 42.886 | 18.031 | -0.513 | 1.00 | 20.90 | C |
| ATOM | 2630 | CD | GLN | B | 97 | 41.549 | 17.837 | 0.182 | 1.00 | 21.44 | C |
| ATOM | 2631 | OE1 | GLN | B | 97 | 41.498 | 17.491 | 1.363 | 1.00 | 21.97 | O |
| ATOM | 2632 | NE2 | GLN | B | 97 | 40.464 | 18.059 | -0.550 | 1.00 | 21.49 | N |
| ATOM | 2633 | N | LEU | B | 98 | 45.104 | 20.484 | -1.661 | 1.00 | 19.76 | N |
| ATOM | 2634 | CA | LEU | B | 98 | 44.974 | 21.882 | -2.038 | 1.00 | 19.64 | C |
| ATOM | 2635 | C | LEU | B | 98 | 43.578 | 22.392 | -1.695 | 1.00 | 19.59 | C |

FIG. 4RR

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2636 | O | LEU | B | 98 | 42.576 | 21.739 | -1.997 | 1.00 | 19.42 | O |
| ATOM | 2637 | CB | LEU | B | 98 | 45.263 | 22.058 | -3.531 | 1.00 | 19.59 | C |
| ATOM | 2638 | CG | LEU | B | 98 | 45.305 | 23.465 | -4.128 | 1.00 | 19.53 | C |
| ATOM | 2639 | CD1 | LEU | B | 98 | 46.346 | 24.340 | -3.444 | 1.00 | 19.49 | C |
| ATOM | 2640 | CD2 | LEU | B | 98 | 45.586 | 23.362 | -5.615 | 1.00 | 20.14 | C |
| ATOM | 2641 | N | MET | B | 99 | 43.527 | 23.555 | -1.052 | 1.00 | 19.48 | N |
| ATOM | 2642 | CA | MET | B | 99 | 42.266 | 24.182 | -0.682 | 1.00 | 19.59 | C |
| ATOM | 2643 | C | MET | B | 99 | 42.120 | 25.515 | -1.422 | 1.00 | 19.36 | C |
| ATOM | 2644 | O | MET | B | 99 | 42.769 | 26.504 | -1.068 | 1.00 | 19.21 | O |
| ATOM | 2645 | CB | MET | B | 99 | 42.170 | 24.369 | 0.840 | 1.00 | 19.83 | C |
| ATOM | 2646 | CG | MET | B | 99 | 42.422 | 23.094 | 1.647 | 1.00 | 20.31 | C |
| ATOM | 2647 | SD | MET | B | 99 | 40.915 | 22.226 | 2.130 | 1.00 | 21.60 | S |
| ATOM | 2648 | CE | MET | B | 99 | 41.579 | 20.613 | 2.522 | 1.00 | 22.18 | C |
| ATOM | 2649 | N | PRO | B | 100 | 41.279 | 25.529 | -2.458 | 1.00 | 19.09 | N |
| ATOM | 2650 | CA | PRO | B | 100 | 41.118 | 26.701 | -3.328 | 1.00 | 18.91 | C |
| ATOM | 2651 | C | PRO | B | 100 | 40.550 | 27.939 | -2.636 | 1.00 | 18.85 | C |
| ATOM | 2652 | O | PRO | B | 100 | 40.681 | 29.030 | -3.188 | 1.00 | 18.91 | O |
| ATOM | 2653 | CB | PRO | B | 100 | 40.135 | 26.207 | -4.394 | 1.00 | 18.90 | C |
| ATOM | 2654 | CG | PRO | B | 100 | 39.400 | 25.101 | -3.742 | 1.00 | 18.85 | C |
| ATOM | 2655 | CD | PRO | B | 100 | 40.420 | 24.410 | -2.888 | 1.00 | 19.12 | C |
| ATOM | 2656 | N | PHE | B | 101 | 39.943 | 27.779 | -1.462 | 1.00 | 18.69 | N |
| ATOM | 2657 | CA | PHE | B | 101 | 39.309 | 28.902 | -0.769 | 1.00 | 18.46 | C |
| ATOM | 2658 | C | PHE | B | 101 | 40.204 | 29.585 | 0.273 | 1.00 | 18.39 | C |
| ATOM | 2659 | O | PHE | B | 101 | 39.830 | 30.615 | 0.838 | 1.00 | 18.52 | O |
| ATOM | 2660 | CB | PHE | B | 101 | 37.963 | 28.478 | -0.169 | 1.00 | 18.51 | C |
| ATOM | 2661 | CG | PHE | B | 101 | 37.016 | 27.882 | -1.173 | 1.00 | 18.48 | C |
| ATOM | 2662 | CD1 | PHE | B | 101 | 36.847 | 28.467 | -2.430 | 1.00 | 18.67 | C |
| ATOM | 2663 | CE1 | PHE | B | 101 | 35.979 | 27.912 | -3.365 | 1.00 | 18.71 | C |
| ATOM | 2664 | CZ | PHE | B | 101 | 35.270 | 26.760 | -3.049 | 1.00 | 18.60 | C |
| ATOM | 2665 | CE2 | PHE | B | 101 | 35.431 | 26.169 | -1.801 | 1.00 | 18.57 | C |
| ATOM | 2666 | CD2 | PHE | B | 101 | 36.301 | 26.731 | -0.871 | 1.00 | 18.34 | C |
| ATOM | 2667 | N | GLY | B | 102 | 41.379 | 29.008 | 0.517 | 1.00 | 18.15 | N |
| ATOM | 2668 | CA | GLY | B | 102 | 42.400 | 29.636 | 1.338 | 1.00 | 17.73 | C |
| ATOM | 2669 | C | GLY | B | 102 | 42.191 | 29.539 | 2.834 | 1.00 | 17.54 | C |
| ATOM | 2670 | O | GLY | B | 102 | 41.487 | 28.649 | 3.318 | 1.00 | 17.50 | O |
| ATOM | 2671 | N | CYS | B | 103 | 42.813 | 30.464 | 3.563 | 1.00 | 17.35 | N |
| ATOM | 2672 | CA | CYS | B | 103 | 42.757 | 30.482 | 5.025 | 1.00 | 17.23 | C |
| ATOM | 2673 | C | CYS | B | 103 | 41.559 | 31.265 | 5.561 | 1.00 | 17.28 | C |
| ATOM | 2674 | O | CYS | B | 103 | 40.886 | 31.978 | 4.814 | 1.00 | 17.12 | O |
| ATOM | 2675 | CB | CYS | B | 103 | 44.072 | 31.015 | 5.616 | 1.00 | 17.32 | C |
| ATOM | 2676 | SG | CYS | B | 103 | 44.527 | 32.701 | 5.135 | 1.00 | 16.78 | S |
| ATOM | 2677 | N | LEU | B | 104 | 41.302 | 31.121 | 6.860 | 1.00 | 17.44 | N |
| ATOM | 2678 | CA | LEU | B | 104 | 40.159 | 31.757 | 7.514 | 1.00 | 17.62 | C |
| ATOM | 2679 | C | LEU | B | 104 | 40.385 | 33.242 | 7.813 | 1.00 | 17.78 | C |
| ATOM | 2680 | O | LEU | B | 104 | 39.432 | 34.021 | 7.834 | 1.00 | 17.86 | O |
| ATOM | 2681 | CB | LEU | B | 104 | 39.785 | 31.000 | 8.795 | 1.00 | 17.54 | C |
| ATOM | 2682 | CG | LEU | B | 104 | 38.447 | 31.275 | 9.495 | 1.00 | 17.46 | C |
| ATOM | 2683 | CD1 | LEU | B | 104 | 37.259 | 31.217 | 8.536 | 1.00 | 17.14 | C |
| ATOM | 2684 | CD2 | LEU | B | 104 | 38.257 | 30.298 | 10.651 | 1.00 | 17.22 | C |
| ATOM | 2685 | N | LEU | B | 105 | 41.641 | 33.621 | 8.048 | 1.00 | 17.91 | N |
| ATOM | 2686 | CA | LEU | B | 105 | 42.006 | 35.017 | 8.290 | 1.00 | 18.02 | C |
| ATOM | 2687 | C | LEU | B | 105 | 41.674 | 35.917 | 7.092 | 1.00 | 18.22 | C |
| ATOM | 2688 | O | LEU | B | 105 | 41.106 | 36.995 | 7.265 | 1.00 | 18.43 | O |
| ATOM | 2689 | CB | LEU | B | 105 | 43.491 | 35.135 | 8.662 | 1.00 | 17.98 | C |
| ATOM | 2690 | CG | LEU | B | 105 | 44.044 | 36.524 | 9.002 | 1.00 | 17.89 | C |
| ATOM | 2691 | CD1 | LEU | B | 105 | 43.593 | 36.980 | 10.387 | 1.00 | 18.20 | C |
| ATOM | 2692 | CD2 | LEU | B | 105 | 45.560 | 36.542 | 8.899 | 1.00 | 17.28 | C |
| ATOM | 2693 | N | ASP | B | 106 | 42.027 | 35.477 | 5.885 | 1.00 | 18.14 | N |
| ATOM | 2694 | CA | ASP | B | 106 | 41.687 | 36.217 | 4.673 | 1.00 | 18.08 | C |
| ATOM | 2695 | C | ASP | B | 106 | 40.173 | 36.213 | 4.431 | 1.00 | 18.19 | C |

FIG. 4SS

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|-------|------|-------|---|
| ATOM | 2696 | O | ASP | B | 106 | 39.610 | 37.213 | 3.982 | 1.00 | 18.20 | O |
| ATOM | 2697 | CB | ASP | B | 106 | 42.437 | 35.661 | 3.457 | 1.00 | 18.06 | C |
| ATOM | 2698 | CG | ASP | B | 106 | 43.957 | 35.828 | 3.565 | 1.00 | 18.47 | C |
| ATOM | 2699 | OD1 | ASP | B | 106 | 44.442 | 36.529 | 4.481 | 1.00 | 18.85 | O |
| ATOM | 2700 | OD2 | ASP | B | 106 | 44.754 | 35.285 | 2.773 | 1.00 | 18.03 | O |
| ATOM | 2701 | N | TYR | B | 107 | 39.521 | 35.095 | 4.750 | 1.00 | 18.27 | N |
| ATOM | 2702 | CA | TYR | B | 107 | 38.073 | 34.971 | 4.586 | 1.00 | 18.25 | C |
| ATOM | 2703 | C | TYR | B | 107 | 37.295 | 35.953 | 5.473 | 1.00 | 18.32 | C |
| ATOM | 2704 | O | TYR | B | 107 | 36.343 | 36.584 | 5.005 | 1.00 | 18.20 | O |
| ATOM | 2705 | CB | TYR | B | 107 | 37.601 | 33.528 | 4.822 | 1.00 | 18.06 | C |
| ATOM | 2706 | CG | TYR | B | 107 | 36.121 | 33.329 | 4.554 | 1.00 | 18.06 | C |
| ATOM | 2707 | CD1 | TYR | B | 107 | 35.656 | 33.042 | 3.271 | 1.00 | 17.84 | C |
| ATOM | 2708 | CE1 | TYR | B | 107 | 34.294 | 32.874 | 3.022 | 1.00 | 17.97 | C |
| ATOM | 2709 | CZ | TYR | B | 107 | 33.385 | 32.995 | 4.066 | 1.00 | 17.63 | C |
| ATOM | 2710 | OH | TYR | B | 107 | 32.038 | 32.829 | 3.831 | 1.00 | 17.31 | O |
| ATOM | 2711 | CE2 | TYR | B | 107 | 33.824 | 33.282 | 5.346 | 1.00 | 17.32 | C |
| ATOM | 2712 | CD2 | TYR | B | 107 | 35.183 | 33.447 | 5.584 | 1.00 | 17.82 | C |
| ATOM | 2713 | N | VAL | B | 108 | 37.699 | 36.078 | 6.739 | 1.00 | 18.40 | N |
| ATOM | 2714 | CA | VAL | B | 108 | 37.060 | 37.025 | 7.661 | 1.00 | 18.57 | C |
| ATOM | 2715 | C | VAL | B | 108 | 37.369 | 38.479 | 7.306 | 1.00 | 18.67 | C |
| ATOM | 2716 | O | VAL | B | 108 | 36.564 | 39.369 | 7.571 | 1.00 | 18.65 | O |
| ATOM | 2717 | CB | VAL | B | 108 | 37.368 | 36.744 | 9.173 | 1.00 | 18.53 | C |
| ATOM | 2718 | CG1 | VAL | B | 108 | 36.831 | 35.381 | 9.600 | 1.00 | 18.69 | C |
| ATOM | 2719 | CG2 | VAL | B | 108 | 38.852 | 36.874 | 9.494 | 1.00 | 18.02 | C |
| ATOM | 2720 | N | ARG | B | 109 | 38.534 | 38.703 | 6.705 | 1.00 | 18.99 | N |
| ATOM | 2721 | CA | ARG | B | 109 | 38.936 | 40.024 | 6.241 | 1.00 | 19.46 | C |
| ATOM | 2722 | C | ARG | B | 109 | 38.146 | 40.438 | 4.999 | 1.00 | 20.04 | C |
| ATOM | 2723 | O | ARG | B | 109 | 37.858 | 41.618 | 4.804 | 1.00 | 20.13 | O |
| ATOM | 2724 | CB | ARG | B | 109 | 40.435 | 40.040 | 5.940 | 1.00 | 19.30 | C |
| ATOM | 2725 | CG | ARG | B | 109 | 41.311 | 40.248 | 7.162 | 1.00 | 18.84 | C |
| ATOM | 2726 | CD | ARG | B | 109 | 42.798 | 40.238 | 6.866 | 1.00 | 18.38 | C |
| ATOM | 2727 | NE | ARG | B | 109 | 43.594 | 40.289 | 8.090 | 1.00 | 18.34 | N |
| ATOM | 2728 | CZ | ARG | B | 109 | 44.919 | 40.184 | 8.140 | 1.00 | 18.12 | C |
| ATOM | 2729 | NH1 | ARG | B | 109 | 45.631 | 40.019 | 7.030 | 1.00 | 17.70 | N |
| ATOM | 2730 | NH2 | ARG | B | 109 | 45.536 | 40.243 | 9.312 | 1.00 | 17.84 | N |
| ATOM | 2731 | N | GLU | B | 110 | 37.794 | 39.458 | 4.171 | 1.00 | 20.87 | N |
| ATOM | 2732 | CA | GLU | B | 110 | 37.071 | 39.709 | 2.928 | 1.00 | 21.60 | C |
| ATOM | 2733 | C | GLU | B | 110 | 35.569 | 39.876 | 3.145 | 1.00 | 22.25 | C |
| ATOM | 2734 | O | GLU | B | 110 | 34.916 | 40.624 | 2.417 | 1.00 | 22.54 | O |
| ATOM | 2735 | CB | GLU | B | 110 | 37.334 | 38.589 | 1.921 | 1.00 | 21.52 | C |
| ATOM | 2736 | N | HIS | B | 111 | 35.027 | 39.183 | 4.145 | 1.00 | 22.82 | N |
| ATOM | 2737 | CA | HIS | B | 111 | 33.587 | 39.193 | 4.396 | 1.00 | 23.38 | C |
| ATOM | 2738 | C | HIS | B | 111 | 33.210 | 39.779 | 5.761 | 1.00 | 23.75 | C |
| ATOM | 2739 | O | HIS | B | 111 | 32.297 | 39.284 | 6.425 | 1.00 | 24.02 | O |
| ATOM | 2740 | CB | HIS | B | 111 | 33.013 | 37.783 | 4.237 | 1.00 | 23.42 | C |
| ATOM | 2741 | CG | HIS | B | 111 | 33.257 | 37.181 | 2.890 | 1.00 | 23.81 | C |
| ATOM | 2742 | ND1 | HIS | B | 111 | 34.409 | 36.490 | 2.584 | 1.00 | 24.33 | N |
| ATOM | 2743 | CE1 | HIS | B | 111 | 34.353 | 36.079 | 1.330 | 1.00 | 24.04 | C |
| ATOM | 2744 | NE2 | HIS | B | 111 | 33.204 | 36.475 | 0.812 | 1.00 | 23.96 | N |
| ATOM | 2745 | CD2 | HIS | B | 111 | 32.501 | 37.168 | 1.767 | 1.00 | 24.20 | C |
| ATOM | 2746 | N | LYS | B | 112 | 33.902 | 40.846 | 6.161 | 1.00 | 24.06 | N |
| ATOM | 2747 | CA | LYS | B | 112 | 33.662 | 41.512 | 7.443 | 1.00 | 24.23 | C |
| ATOM | 2748 | C | LYS | B | 112 | 32.180 | 41.805 | 7.688 | 1.00 | 24.53 | C |
| ATOM | 2749 | O | LYS | B | 112 | 31.649 | 41.498 | 8.760 | 1.00 | 24.80 | O |
| ATOM | 2750 | CB | LYS | B | 112 | 34.458 | 42.818 | 7.534 | 1.00 | 24.18 | C |
| ATOM | 2751 | CG | LYS | B | 112 | 35.961 | 42.643 | 7.656 | 1.00 | 24.18 | C |
| ATOM | 2752 | N | ASP | B | 113 | 31.519 | 42.386 | 6.688 | 1.00 | 24.57 | N |
| ATOM | 2753 | CA | ASP | B | 113 | 30.127 | 42.813 | 6.826 | 1.00 | 24.85 | C |
| ATOM | 2754 | C | ASP | B | 113 | 29.096 | 41.740 | 6.472 | 1.00 | 24.82 | C |
| ATOM | 2755 | O | ASP | B | 113 | 27.902 | 42.034 | 6.378 | 1.00 | 25.13 | O |

FIG. 4TT

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2756 | N | ASN | B | 114 | 29.552 | 40.503 | 6.294 | 1.00 | 24.62 | N |
| ATOM | 2757 | CA | ASN | B | 114 | 28.686 | 39.418 | 5.836 | 1.00 | 24.36 | C |
| ATOM | 2758 | C | ASN | B | 114 | 28.683 | 38.182 | 6.739 | 1.00 | 24.12 | C |
| ATOM | 2759 | O | ASN | B | 114 | 27.770 | 37.358 | 6.668 | 1.00 | 24.02 | O |
| ATOM | 2760 | CB | ASN | B | 114 | 29.058 | 39.021 | 4.407 | 1.00 | 24.60 | C |
| ATOM | 2761 | N | ILE | B | 115 | 29.702 | 38.056 | 7.584 | 1.00 | 23.83 | N |
| ATOM | 2762 | CA | ILE | B | 115 | 29.812 | 36.907 | 8.477 | 1.00 | 23.51 | C |
| ATOM | 2763 | C | ILE | B | 115 | 28.903 | 37.056 | 9.700 | 1.00 | 23.34 | C |
| ATOM | 2764 | O | ILE | B | 115 | 28.963 | 38.059 | 10.416 | 1.00 | 23.07 | O |
| ATOM | 2765 | CB | ILE | B | 115 | 31.288 | 36.659 | 8.882 | 1.00 | 23.39 | C |
| ATOM | 2766 | CG1 | ILE | B | 115 | 32.126 | 36.332 | 7.643 | 1.00 | 23.15 | C |
| ATOM | 2767 | CD1 | ILE | B | 115 | 33.604 | 36.605 | 7.801 | 1.00 | 23.01 | C |
| ATOM | 2768 | CG2 | ILE | B | 115 | 31.388 | 35.514 | 9.890 | 1.00 | 23.54 | C |
| ATOM | 2769 | N | GLY | B | 116 | 28.056 | 36.051 | 9.915 | 1.00 | 23.22 | N |
| ATOM | 2770 | CA | GLY | B | 116 | 27.140 | 36.032 | 11.042 | 1.00 | 23.09 | C |
| ATOM | 2771 | C | GLY | B | 116 | 27.760 | 35.433 | 12.290 | 1.00 | 23.12 | C |
| ATOM | 2772 | O | GLY | B | 116 | 28.814 | 34.790 | 12.225 | 1.00 | 23.04 | O |
| ATOM | 2773 | N | SER | B | 117 | 27.098 | 35.646 | 13.426 | 1.00 | 22.96 | N |
| ATOM | 2774 | CA | SER | B | 117 | 27.555 | 35.137 | 14.720 | 1.00 | 22.87 | C |
| ATOM | 2775 | C | SER | B | 117 | 27.519 | 33.612 | 14.810 | 1.00 | 22.68 | C |
| ATOM | 2776 | O | SER | B | 117 | 28.327 | 33.014 | 15.523 | 1.00 | 22.86 | O |
| ATOM | 2777 | CB | SER | B | 117 | 26.744 | 35.750 | 15.866 | 1.00 | 22.90 | C |
| ATOM | 2778 | OG | SER | B | 117 | 25.435 | 36.097 | 15.447 | 1.00 | 23.42 | O |
| ATOM | 2779 | N | GLN | B | 118 | 26.586 | 32.989 | 14.092 | 1.00 | 22.42 | N |
| ATOM | 2780 | CA | GLN | B | 118 | 26.490 | 31.530 | 14.052 | 1.00 | 22.18 | C |
| ATOM | 2781 | C | GLN | B | 118 | 27.730 | 30.904 | 13.409 | 1.00 | 21.88 | C |
| ATOM | 2782 | O | GLN | B | 118 | 28.264 | 29.917 | 13.919 | 1.00 | 21.95 | O |
| ATOM | 2783 | CB | GLN | B | 118 | 25.207 | 31.078 | 13.338 | 1.00 | 22.27 | C |
| ATOM | 2784 | CG | GLN | B | 118 | 24.991 | 29.558 | 13.278 | 1.00 | 22.98 | C |
| ATOM | 2785 | CD | GLN | B | 118 | 24.809 | 28.919 | 14.649 | 1.00 | 23.82 | C |
| ATOM | 2786 | OE1 | GLN | B | 118 | 25.787 | 28.617 | 15.335 | 1.00 | 24.34 | O |
| ATOM | 2787 | NE2 | GLN | B | 118 | 23.559 | 28.705 | 15.044 | 1.00 | 24.11 | N |
| ATOM | 2788 | N | TYR | B | 119 | 28.183 | 31.485 | 12.300 | 1.00 | 21.29 | N |
| ATOM | 2789 | CA | TYR | B | 119 | 29.392 | 31.030 | 11.621 | 1.00 | 20.92 | C |
| ATOM | 2790 | C | TYR | B | 119 | 30.635 | 31.274 | 12.472 | 1.00 | 20.67 | C |
| ATOM | 2791 | O | TYR | B | 119 | 31.511 | 30.414 | 12.562 | 1.00 | 20.72 | O |
| ATOM | 2792 | CB | TYR | B | 119 | 29.544 | 31.728 | 10.267 | 1.00 | 21.08 | C |
| ATOM | 2793 | CG | TYR | B | 119 | 28.788 | 31.067 | 9.134 | 1.00 | 21.26 | C |
| ATOM | 2794 | CD1 | TYR | B | 119 | 29.408 | 30.127 | 8.315 | 1.00 | 21.56 | C |
| ATOM | 2795 | CE1 | TYR | B | 119 | 28.720 | 29.517 | 7.268 | 1.00 | 21.68 | C |
| ATOM | 2796 | CZ | TYR | B | 119 | 27.397 | 29.851 | 7.033 | 1.00 | 21.81 | C |
| ATOM | 2797 | OH | TYR | B | 119 | 26.716 | 29.251 | 5.998 | 1.00 | 22.03 | O |
| ATOM | 2798 | CE2 | TYR | B | 119 | 26.758 | 30.784 | 7.833 | 1.00 | 21.73 | C |
| ATOM | 2799 | CD2 | TYR | B | 119 | 27.455 | 31.388 | 8.877 | 1.00 | 21.51 | C |
| ATOM | 2800 | N | LEU | B | 120 | 30.699 | 32.445 | 13.101 | 1.00 | 20.39 | N |
| ATOM | 2801 | CA | LEU | B | 120 | 31.836 | 32.818 | 13.938 | 1.00 | 20.10 | C |
| ATOM | 2802 | C | LEU | B | 120 | 32.042 | 31.841 | 15.092 | 1.00 | 20.02 | C |
| ATOM | 2803 | O | LEU | B | 120 | 33.153 | 31.356 | 15.309 | 1.00 | 19.87 | O |
| ATOM | 2804 | CB | LEU | B | 120 | 31.675 | 34.246 | 14.471 | 1.00 | 19.95 | C |
| ATOM | 2805 | CG | LEU | B | 120 | 32.001 | 35.410 | 13.528 | 1.00 | 19.91 | C |
| ATOM | 2806 | CD1 | LEU | B | 120 | 31.516 | 36.726 | 14.116 | 1.00 | 19.65 | C |
| ATOM | 2807 | CD2 | LEU | B | 120 | 33.491 | 35.488 | 13.185 | 1.00 | 19.49 | C |
| ATOM | 2808 | N | LEU | B | 121 | 30.964 | 31.546 | 15.814 | 1.00 | 20.01 | N |
| ATOM | 2809 | CA | LEU | B | 121 | 31.026 | 30.660 | 16.975 | 1.00 | 19.95 | C |
| ATOM | 2810 | C | LEU | B | 121 | 31.207 | 29.194 | 16.586 | 1.00 | 19.77 | C |
| ATOM | 2811 | O | LEU | B | 121 | 31.815 | 28.423 | 17.329 | 1.00 | 19.76 | O |
| ATOM | 2812 | CB | LEU | B | 121 | 29.791 | 30.840 | 17.868 | 1.00 | 19.94 | C |
| ATOM | 2813 | CG | LEU | B | 121 | 29.656 | 32.194 | 18.576 | 1.00 | 19.90 | C |
| ATOM | 2814 | CD1 | LEU | B | 121 | 28.244 | 32.388 | 19.099 | 1.00 | 20.14 | C |
| ATOM | 2815 | CD2 | LEU | B | 121 | 30.665 | 32.358 | 19.705 | 1.00 | 19.57 | C |

FIG. 4UU

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2816 | N | ASN | B | 122 | 30.683 | 28.821 | 15.420 | 1.00 | 19.62 | N |
| ATOM | 2817 | CA | ASN | B | 122 | 30.844 | 27.468 | 14.895 | 1.00 | 19.45 | C |
| ATOM | 2818 | C | ASN | B | 122 | 32.290 | 27.157 | 14.528 | 1.00 | 19.12 | C |
| ATOM | 2819 | O | ASN | B | 122 | 32.768 | 26.045 | 14.756 | 1.00 | 18.91 | O |
| ATOM | 2820 | CB | ASN | B | 122 | 29.928 | 27.238 | 13.692 | 1.00 | 19.72 | C |
| ATOM | 2821 | CG | ASN | B | 122 | 28.632 | 26.544 | 14.074 | 1.00 | 20.61 | C |
| ATOM | 2822 | OD1 | ASN | B | 122 | 28.647 | 25.484 | 14.706 | 1.00 | 21.87 | O |
| ATOM | 2823 | ND2 | ASN | B | 122 | 27.503 | 27.139 | 13.695 | 1.00 | 20.28 | N |
| ATOM | 2824 | N | TRP | B | 123 | 32.980 | 28.148 | 13.966 | 1.00 | 18.74 | N |
| ATOM | 2825 | CA | TRP | B | 123 | 34.396 | 28.020 | 13.643 | 1.00 | 18.47 | C |
| ATOM | 2826 | C | TRP | B | 123 | 35.207 | 27.767 | 14.908 | 1.00 | 18.22 | C |
| ATOM | 2827 | O | TRP | B | 123 | 36.106 | 26.929 | 14.917 | 1.00 | 18.04 | O |
| ATOM | 2828 | CB | TRP | B | 123 | 34.902 | 29.265 | 12.911 | 1.00 | 18.46 | C |
| ATOM | 2829 | CG | TRP | B | 123 | 34.348 | 29.418 | 11.517 | 1.00 | 18.58 | C |
| ATOM | 2830 | CD1 | TRP | B | 123 | 33.917 | 28.418 | 10.687 | 1.00 | 18.75 | C |
| ATOM | 2831 | NE1 | TRP | B | 123 | 33.478 | 28.944 | 9.495 | 1.00 | 18.82 | N |
| ATOM | 2832 | CE2 | TRP | B | 123 | 33.623 | 30.306 | 9.530 | 1.00 | 18.59 | C |
| ATOM | 2833 | CD2 | TRP | B | 123 | 34.169 | 30.640 | 10.791 | 1.00 | 18.39 | C |
| ATOM | 2834 | CE3 | TRP | B | 123 | 34.412 | 31.991 | 11.077 | 1.00 | 18.66 | C |
| ATOM | 2835 | CZ3 | TRP | B | 123 | 34.107 | 32.952 | 10.109 | 1.00 | 18.97 | C |
| ATOM | 2836 | CH2 | TRP | B | 123 | 33.568 | 32.582 | 8.865 | 1.00 | 18.65 | C |
| ATOM | 2837 | CZ2 | TRP | B | 123 | 33.320 | 31.269 | 8.557 | 1.00 | 18.57 | C |
| ATOM | 2838 | N | CYS | B | 124 | 34.856 | 28.479 | 15.976 | 1.00 | 18.17 | N |
| ATOM | 2839 | CA | CYS | B | 124 | 35.486 | 28.312 | 17.282 | 1.00 | 18.10 | C |
| ATOM | 2840 | C | CYS | B | 124 | 35.261 | 26.917 | 17.862 | 1.00 | 18.10 | C |
| ATOM | 2841 | O | CYS | B | 124 | 36.170 | 26.351 | 18.467 | 1.00 | 18.31 | O |
| ATOM | 2842 | CB | CYS | B | 124 | 34.985 | 29.378 | 18.254 | 1.00 | 18.05 | C |
| ATOM | 2843 | SG | CYS | B | 124 | 35.578 | 31.039 | 17.875 | 1.00 | 18.24 | S |
| ATOM | 2844 | N | VAL | B | 125 | 34.056 | 26.374 | 17.671 | 1.00 | 17.86 | N |
| ATOM | 2845 | CA | VAL | B | 125 | 33.742 | 24.999 | 18.066 | 1.00 | 17.67 | C |
| ATOM | 2846 | C | VAL | B | 125 | 34.603 | 24.012 | 17.283 | 1.00 | 17.58 | C |
| ATOM | 2847 | O | VAL | B | 125 | 35.269 | 23.161 | 17.871 | 1.00 | 17.89 | O |
| ATOM | 2848 | CB | VAL | B | 125 | 32.237 | 24.657 | 17.855 | 1.00 | 17.72 | C |
| ATOM | 2849 | CG1 | VAL | B | 125 | 31.971 | 23.165 | 18.067 | 1.00 | 17.40 | C |
| ATOM | 2850 | CG2 | VAL | B | 125 | 31.360 | 25.473 | 18.779 | 1.00 | 17.66 | C |
| ATOM | 2851 | N | GLN | B | 126 | 34.587 | 24.144 | 15.957 | 1.00 | 17.52 | N |
| ATOM | 2852 | CA | GLN | B | 126 | 35.318 | 23.250 | 15.057 | 1.00 | 17.19 | C |
| ATOM | 2853 | C | GLN | B | 126 | 36.829 | 23.275 | 15.298 | 1.00 | 16.88 | C |
| ATOM | 2854 | O | GLN | B | 126 | 37.473 | 22.224 | 15.317 | 1.00 | 16.64 | O |
| ATOM | 2855 | CB | GLN | B | 126 | 34.997 | 23.579 | 13.593 | 1.00 | 17.36 | C |
| ATOM | 2856 | CG | GLN | B | 126 | 33.527 | 23.375 | 13.216 | 1.00 | 17.55 | C |
| ATOM | 2857 | CD | GLN | B | 126 | 33.239 | 23.563 | 11.731 | 1.00 | 17.75 | C |
| ATOM | 2858 | OE1 | GLN | B | 126 | 34.118 | 23.941 | 10.956 | 1.00 | 17.46 | O |
| ATOM | 2859 | NE2 | GLN | B | 126 | 32.003 | 23.291 | 11.335 | 1.00 | 18.32 | N |
| ATOM | 2860 | N | ILE | B | 127 | 37.382 | 24.474 | 15.491 | 1.00 | 16.54 | N |
| ATOM | 2861 | CA | ILE | B | 127 | 38.805 | 24.638 | 15.801 | 1.00 | 16.23 | C |
| ATOM | 2862 | C | ILE | B | 127 | 39.158 | 23.975 | 17.137 | 1.00 | 16.00 | C |
| ATOM | 2863 | O | ILE | B | 127 | 40.196 | 23.321 | 17.262 | 1.00 | 15.76 | O |
| ATOM | 2864 | CB | ILE | B | 127 | 39.214 | 26.137 | 15.788 | 1.00 | 16.20 | C |
| ATOM | 2865 | CG1 | ILE | B | 127 | 39.070 | 26.721 | 14.373 | 1.00 | 16.20 | C |
| ATOM | 2866 | CD1 | ILE | B | 127 | 39.018 | 28.244 | 14.317 | 1.00 | 15.72 | C |
| ATOM | 2867 | CG2 | ILE | B | 127 | 40.647 | 26.318 | 16.293 | 1.00 | 16.04 | C |
| ATOM | 2868 | N | ALA | B | 128 | 38.279 | 24.136 | 18.123 | 1.00 | 15.84 | N |
| ATOM | 2869 | CA | ALA | B | 128 | 38.450 | 23.501 | 19.426 | 1.00 | 15.76 | C |
| ATOM | 2870 | C | ALA | B | 128 | 38.404 | 21.974 | 19.322 | 1.00 | 15.68 | C |
| ATOM | 2871 | O | ALA | B | 128 | 39.105 | 21.281 | 20.056 | 1.00 | 15.52 | O |
| ATOM | 2872 | CB | ALA | B | 128 | 37.406 | 24.009 | 20.409 | 1.00 | 15.66 | C |
| ATOM | 2873 | N | LYS | B | 129 | 37.584 | 21.465 | 18.404 | 1.00 | 15.73 | N |
| ATOM | 2874 | CA | LYS | B | 129 | 37.468 | 20.027 | 18.161 | 1.00 | 15.84 | C |
| ATOM | 2875 | C | LYS | B | 129 | 38.739 | 19.434 | 17.547 | 1.00 | 15.85 | C |

FIG. 4VV

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2876 | O | LYS | B | 129 | 39.167 | 18.345 | 17.926 | 1.00 | 16.07 | O |
| ATOM | 2877 | CB | LYS | B | 129 | 36.263 | 19.728 | 17.268 | 1.00 | 15.82 | C |
| ATOM | 2878 | CG | LYS | B | 129 | 34.967 | 19.531 | 18.029 | 1.00 | 15.93 | C |
| ATOM | 2879 | CD | LYS | B | 129 | 33.783 | 19.410 | 17.084 | 1.00 | 15.72 | C |
| ATOM | 2880 | CE | LYS | B | 129 | 32.476 | 19.362 | 17.858 | 1.00 | 15.83 | C |
| ATOM | 2881 | NZ | LYS | B | 129 | 31.305 | 19.242 | 16.946 | 1.00 | 16.38 | N |
| ATOM | 2882 | N | GLY | B | 130 | 39.331 | 20.154 | 16.600 | 1.00 | 15.93 | N |
| ATOM | 2883 | CA | GLY | B | 130 | 40.568 | 19.727 | 15.972 | 1.00 | 15.97 | C |
| ATOM | 2884 | C | GLY | B | 130 | 41.735 | 19.725 | 16.940 | 1.00 | 16.03 | C |
| ATOM | 2885 | O | GLY | B | 130 | 42.549 | 18.801 | 16.941 | 1.00 | 16.07 | O |
| ATOM | 2886 | N | MET | B | 131 | 41.809 | 20.764 | 17.765 | 1.00 | 16.29 | N |
| ATOM | 2887 | CA | MET | B | 131 | 42.863 | 20.895 | 18.769 | 1.00 | 16.62 | C |
| ATOM | 2888 | C | MET | B | 131 | 42.734 | 19.869 | 19.897 | 1.00 | 16.73 | C |
| ATOM | 2889 | O | MET | B | 131 | 43.746 | 19.394 | 20.423 | 1.00 | 16.84 | O |
| ATOM | 2890 | CB | MET | B | 131 | 42.885 | 22.312 | 19.339 | 1.00 | 16.67 | C |
| ATOM | 2891 | CG | MET | B | 131 | 43.430 | 23.370 | 18.387 | 1.00 | 17.05 | C |
| ATOM | 2892 | SD | MET | B | 131 | 45.008 | 22.951 | 17.585 | 1.00 | 17.91 | S |
| ATOM | 2893 | CE | MET | B | 131 | 46.103 | 22.850 | 18.989 | 1.00 | 17.40 | C |
| ATOM | 2894 | N | ASN | B | 132 | 41.493 | 19.529 | 20.251 | 1.00 | 16.65 | N |
| ATOM | 2895 | CA | ASN | B | 132 | 41.211 | 18.486 | 21.237 | 1.00 | 16.95 | C |
| ATOM | 2896 | C | ASN | B | 132 | 41.600 | 17.092 | 20.742 | 1.00 | 17.17 | C |
| ATOM | 2897 | O | ASN | B | 132 | 42.005 | 16.235 | 21.532 | 1.00 | 17.06 | O |
| ATOM | 2898 | CB | ASN | B | 132 | 39.734 | 18.513 | 21.644 | 1.00 | 17.04 | C |
| ATOM | 2899 | CG | ASN | B | 132 | 39.374 | 17.415 | 22.638 | 1.00 | 17.08 | C |
| ATOM | 2900 | OD1 | ASN | B | 132 | 39.711 | 17.494 | 23.820 | 1.00 | 17.27 | O |
| ATOM | 2901 | ND2 | ASN | B | 132 | 38.688 | 16.385 | 22.158 | 1.00 | 16.77 | N |
| ATOM | 2902 | N | TYR | B | 133 | 41.470 | 16.876 | 19.435 | 1.00 | 17.40 | N |
| ATOM | 2903 | CA | TYR | B | 133 | 41.884 | 15.626 | 18.810 | 1.00 | 17.86 | C |
| ATOM | 2904 | C | TYR | B | 133 | 43.389 | 15.416 | 18.979 | 1.00 | 18.34 | C |
| ATOM | 2905 | O | TYR | B | 133 | 43.836 | 14.308 | 19.280 | 1.00 | 18.24 | O |
| ATOM | 2906 | CB | TYR | B | 133 | 41.493 | 15.605 | 17.323 | 1.00 | 17.73 | C |
| ATOM | 2907 | CG | TYR | B | 133 | 42.120 | 14.470 | 16.538 | 1.00 | 17.62 | C |
| ATOM | 2908 | CD1 | TYR | B | 133 | 41.546 | 13.199 | 16.533 | 1.00 | 17.36 | C |
| ATOM | 2909 | CE1 | TYR | B | 133 | 42.126 | 12.149 | 15.822 | 1.00 | 17.33 | C |
| ATOM | 2910 | CZ | TYR | B | 133 | 43.291 | 12.370 | 15.105 | 1.00 | 17.43 | C |
| ATOM | 2911 | OH | TYR | B | 133 | 43.867 | 11.339 | 14.400 | 1.00 | 17.21 | O |
| ATOM | 2912 | CE2 | TYR | B | 133 | 43.881 | 13.625 | 15.095 | 1.00 | 17.75 | C |
| ATOM | 2913 | CD2 | TYR | B | 133 | 43.295 | 14.667 | 15.810 | 1.00 | 17.67 | C |
| ATOM | 2914 | N | LEU | B | 134 | 44.155 | 16.491 | 18.790 | 1.00 | 19.19 | N |
| ATOM | 2915 | CA | LEU | B | 134 | 45.615 | 16.446 | 18.881 | 1.00 | 19.69 | C |
| ATOM | 2916 | C | LEU | B | 134 | 46.092 | 16.263 | 20.319 | 1.00 | 19.99 | C |
| ATOM | 2917 | O | LEU | B | 134 | 47.029 | 15.506 | 20.563 | 1.00 | 19.99 | O |
| ATOM | 2918 | CB | LEU | B | 134 | 46.251 | 17.700 | 18.260 | 1.00 | 19.75 | C |
| ATOM | 2919 | CG | LEU | B | 134 | 45.903 | 18.102 | 16.819 | 1.00 | 19.96 | C |
| ATOM | 2920 | CD1 | LEU | B | 134 | 46.316 | 19.544 | 16.556 | 1.00 | 20.06 | C |
| ATOM | 2921 | CD2 | LEU | B | 134 | 46.536 | 17.172 | 15.784 | 1.00 | 19.80 | C |
| ATOM | 2922 | N | GLU | B | 135 | 45.446 | 16.947 | 21.265 | 1.00 | 20.49 | N |
| ATOM | 2923 | CA | GLU | B | 135 | 45.793 | 16.813 | 22.682 | 1.00 | 21.01 | C |
| ATOM | 2924 | C | GLU | B | 135 | 45.592 | 15.384 | 23.184 | 1.00 | 21.11 | C |
| ATOM | 2925 | O | GLU | B | 135 | 46.452 | 14.842 | 23.878 | 1.00 | 21.37 | O |
| ATOM | 2926 | CB | GLU | B | 135 | 45.009 | 17.807 | 23.547 | 1.00 | 21.19 | C |
| ATOM | 2927 | CG | GLU | B | 135 | 45.281 | 17.670 | 25.043 | 1.00 | 21.71 | C |
| ATOM | 2928 | CD | GLU | B | 135 | 44.607 | 18.739 | 25.884 | 1.00 | 22.55 | C |
| ATOM | 2929 | OE1 | GLU | B | 135 | 44.984 | 18.880 | 27.068 | 1.00 | 23.01 | O |
| ATOM | 2930 | OE2 | GLU | B | 135 | 43.703 | 19.437 | 25.373 | 1.00 | 22.88 | O |
| ATOM | 2931 | N | ASP | B | 136 | 44.461 | 14.779 | 22.822 | 1.00 | 21.26 | N |
| ATOM | 2932 | CA | ASP | B | 136 | 44.170 | 13.384 | 23.156 | 1.00 | 21.22 | C |
| ATOM | 2933 | C | ASP | B | 136 | 45.202 | 12.441 | 22.548 | 1.00 | 21.29 | C |
| ATOM | 2934 | O | ASP | B | 136 | 45.417 | 11.331 | 23.041 | 1.00 | 21.52 | O |
| ATOM | 2935 | CB | ASP | B | 136 | 42.776 | 13.001 | 22.664 | 1.00 | 21.12 | C |

FIG. 4WW

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2936 | CG | ASP | B | 136 | 41.676 | 13.506 | 23.571 | 1.00 | 21.19 | C |
| ATOM | 2937 | OD1 | ASP | B | 136 | 40.496 | 13.219 | 23.274 | 1.00 | 21.35 | O |
| ATOM | 2938 | OD2 | ASP | B | 136 | 41.888 | 14.192 | 24.598 | 1.00 | 20.89 | O |
| ATOM | 2939 | N | ARG | B | 137 | 45.832 | 12.901 | 21.473 | 1.00 | 21.22 | N |
| ATOM | 2940 | CA | ARG | B | 137 | 46.881 | 12.156 | 20.797 | 1.00 | 21.19 | C |
| ATOM | 2941 | C | ARG | B | 137 | 48.273 | 12.553 | 21.287 | 1.00 | 21.50 | C |
| ATOM | 2942 | O | ARG | B | 137 | 49.276 | 12.034 | 20.792 | 1.00 | 21.78 | O |
| ATOM | 2943 | CB | ARG | B | 137 | 46.777 | 12.385 | 19.293 | 1.00 | 21.11 | C |
| ATOM | 2944 | CG | ARG | B | 137 | 45.720 | 11.541 | 18.622 | 1.00 | 20.57 | C |
| ATOM | 2945 | CD | ARG | B | 137 | 46.293 | 10.363 | 17.886 | 1.00 | 20.38 | C |
| ATOM | 2946 | NE | ARG | B | 137 | 46.161 | 10.528 | 16.448 | 1.00 | 20.23 | N |
| ATOM | 2947 | CZ | ARG | B | 137 | 47.039 | 10.101 | 15.555 | 1.00 | 20.44 | C |
| ATOM | 2948 | NH1 | ARG | B | 137 | 48.146 | 9.475 | 15.933 | 1.00 | 20.25 | N |
| ATOM | 2949 | NH2 | ARG | B | 137 | 46.805 | 10.304 | 14.270 | 1.00 | 21.11 | N |
| ATOM | 2950 | N | ARG | B | 138 | 48.323 | 13.470 | 22.258 | 1.00 | 21.46 | N |
| ATOM | 2951 | CA | ARG | B | 138 | 49.576 | 14.008 | 22.800 | 1.00 | 21.41 | C |
| ATOM | 2952 | C | ARG | B | 138 | 50.406 | 14.722 | 21.726 | 1.00 | 21.38 | C |
| ATOM | 2953 | O | ARG | B | 138 | 51.634 | 14.597 | 21.682 | 1.00 | 21.48 | O |
| ATOM | 2954 | CB | ARG | B | 138 | 50.395 | 12.914 | 23.507 | 1.00 | 21.43 | C |
| ATOM | 2955 | CG | ARG | B | 138 | 49.737 | 12.352 | 24.760 | 1.00 | 21.40 | C |
| ATOM | 2956 | N | LEU | B | 139 | 49.714 | 15.477 | 20.874 | 1.00 | 21.20 | N |
| ATOM | 2957 | CA | LEU | B | 139 | 50.327 | 16.223 | 19.779 | 1.00 | 20.98 | C |
| ATOM | 2958 | C | LEU | B | 139 | 50.226 | 17.729 | 20.023 | 1.00 | 20.89 | C |
| ATOM | 2959 | O | LEU | B | 139 | 49.163 | 18.237 | 20.394 | 1.00 | 21.12 | O |
| ATOM | 2960 | CB | LEU | B | 139 | 49.643 | 15.864 | 18.455 | 1.00 | 21.10 | C |
| ATOM | 2961 | CG | LEU | B | 139 | 50.241 | 14.808 | 17.511 | 1.00 | 21.43 | C |
| ATOM | 2962 | CD1 | LEU | B | 139 | 50.470 | 13.462 | 18.197 | 1.00 | 21.52 | C |
| ATOM | 2963 | CD2 | LEU | B | 139 | 49.332 | 14.626 | 16.303 | 1.00 | 21.15 | C |
| ATOM | 2964 | N | VAL | B | 140 | 51.338 | 18.433 | 19.817 | 1.00 | 20.57 | N |
| ATOM | 2965 | CA | VAL | B | 140 | 51.393 | 19.887 | 19.974 | 1.00 | 20.16 | C |
| ATOM | 2966 | C | VAL | B | 140 | 51.525 | 20.560 | 18.608 | 1.00 | 19.92 | C |
| ATOM | 2967 | O | VAL | B | 140 | 52.339 | 20.153 | 17.780 | 1.00 | 20.12 | O |
| ATOM | 2968 | CB | VAL | B | 140 | 52.564 | 20.336 | 20.898 | 1.00 | 20.16 | C |
| ATOM | 2969 | CG1 | VAL | B | 140 | 52.452 | 21.824 | 21.241 | 1.00 | 20.11 | C |
| ATOM | 2970 | CG2 | VAL | B | 140 | 52.607 | 19.504 | 22.173 | 1.00 | 19.85 | C |
| ATOM | 2971 | N | HIS | B | 141 | 50.714 | 21.587 | 18.380 | 1.00 | 19.72 | N |
| ATOM | 2972 | CA | HIS | B | 141 | 50.731 | 22.321 | 17.118 | 1.00 | 19.24 | C |
| ATOM | 2973 | C | HIS | B | 141 | 51.921 | 23.272 | 17.024 | 1.00 | 18.97 | C |
| ATOM | 2974 | O | HIS | B | 141 | 52.681 | 23.217 | 16.055 | 1.00 | 18.93 | O |
| ATOM | 2975 | CB | HIS | B | 141 | 49.421 | 23.084 | 16.917 | 1.00 | 19.26 | C |
| ATOM | 2976 | CG | HIS | B | 141 | 49.247 | 23.616 | 15.531 | 1.00 | 19.28 | C |
| ATOM | 2977 | ND1 | HIS | B | 141 | 48.259 | 23.169 | 14.682 | 1.00 | 19.51 | N |
| ATOM | 2978 | CE1 | HIS | B | 141 | 48.348 | 23.812 | 13.532 | 1.00 | 19.59 | C |
| ATOM | 2979 | NE2 | HIS | B | 141 | 49.361 | 24.656 | 13.602 | 1.00 | 19.42 | N |
| ATOM | 2980 | CD2 | HIS | B | 141 | 49.940 | 24.553 | 14.842 | 1.00 | 19.11 | C |
| ATOM | 2981 | N | ARG | B | 142 | 52.056 | 24.147 | 18.025 | 1.00 | 18.49 | N |
| ATOM | 2982 | CA | ARG | B | 142 | 53.168 | 25.101 | 18.142 | 1.00 | 18.18 | C |
| ATOM | 2983 | C | ARG | B | 142 | 53.036 | 26.365 | 17.282 | 1.00 | 17.91 | C |
| ATOM | 2984 | O | ARG | B | 142 | 53.696 | 27.373 | 17.553 | 1.00 | 17.68 | O |
| ATOM | 2985 | CB | ARG | B | 142 | 54.504 | 24.439 | 17.779 | 1.00 | 18.23 | C |
| ATOM | 2986 | CG | ARG | B | 142 | 55.068 | 23.552 | 18.868 | 1.00 | 18.68 | C |
| ATOM | 2987 | CD | ARG | B | 142 | 56.479 | 23.076 | 18.603 | 1.00 | 19.06 | C |
| ATOM | 2988 | NE | ARG | B | 142 | 56.808 | 21.913 | 19.417 | 1.00 | 20.04 | N |
| ATOM | 2989 | CZ | ARG | B | 142 | 58.033 | 21.588 | 19.806 | 1.00 | 20.63 | C |
| ATOM | 2990 | NH1 | ARG | B | 142 | 58.223 | 20.506 | 20.553 | 1.00 | 20.97 | N |
| ATOM | 2991 | NH2 | ARG | B | 142 | 59.072 | 22.336 | 19.457 | 1.00 | 20.60 | N |
| ATOM | 2992 | N | ASP | B | 143 | 52.088 | 26.435 | 16.410 | 1.00 | 17.56 | N |
| ATOM | 2993 | CA | ASP | B | 143 | 51.905 | 27.568 | 15.505 | 1.00 | 17.29 | C |
| ATOM | 2994 | C | ASP | B | 143 | 50.438 | 27.760 | 15.080 | 1.00 | 17.09 | C |
| ATOM | 2995 | O | ASP | B | 143 | 50.131 | 27.927 | 13.897 | 1.00 | 16.75 | O |

FIG. 4XX

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2996 | CB | ASP | B | 143 | 52.833 | 27.410 | 14.294 | 1.00 | 17.20 | C |
| ATOM | 2997 | CG | ASP | B | 143 | 52.791 | 28.598 | 13.351 | 1.00 | 17.40 | C |
| ATOM | 2998 | OD1 | ASP | B | 143 | 52.632 | 29.750 | 13.809 | 1.00 | 17.98 | O |
| ATOM | 2999 | OD2 | ASP | B | 143 | 52.910 | 28.466 | 12.118 | 1.00 | 17.68 | O |
| ATOM | 3000 | N | LEU | B | 144 | 49.533 | 27.736 | 16.055 | 1.00 | 16.94 | N |
| ATOM | 3001 | CA | LEU | B | 144 | 48.114 | 27.924 | 15.771 | 1.00 | 16.92 | C |
| ATOM | 3002 | C | LEU | B | 144 | 47.790 | 29.404 | 15.589 | 1.00 | 16.96 | C |
| ATOM | 3003 | O | LEU | B | 144 | 48.176 | 30.245 | 16.405 | 1.00 | 17.13 | O |
| ATOM | 3004 | CB | LEU | B | 144 | 47.235 | 27.291 | 16.859 | 1.00 | 16.90 | C |
| ATOM | 3005 | CG | LEU | B | 144 | 45.706 | 27.351 | 16.717 | 1.00 | 17.00 | C |
| ATOM | 3006 | CD1 | LEU | B | 144 | 45.208 | 26.711 | 15.416 | 1.00 | 17.04 | C |
| ATOM | 3007 | CD2 | LEU | B | 144 | 45.037 | 26.704 | 17.920 | 1.00 | 16.42 | C |
| ATOM | 3008 | N | ALA | B | 145 | 47.094 | 29.702 | 14.496 | 1.00 | 16.70 | N |
| ATOM | 3009 | CA | ALA | B | 145 | 46.692 | 31.057 | 14.144 | 1.00 | 16.53 | C |
| ATOM | 3010 | C | ALA | B | 145 | 45.571 | 30.984 | 13.116 | 1.00 | 16.37 | C |
| ATOM | 3011 | O | ALA | B | 145 | 45.374 | 29.943 | 12.486 | 1.00 | 16.65 | O |
| ATOM | 3012 | CB | ALA | B | 145 | 47.875 | 31.830 | 13.586 | 1.00 | 16.61 | C |
| ATOM | 3013 | N | ALA | B | 146 | 44.841 | 32.084 | 12.943 | 1.00 | 15.84 | N |
| ATOM | 3014 | CA | ALA | B | 146 | 43.747 | 32.135 | 11.975 | 1.00 | 15.60 | C |
| ATOM | 3015 | C | ALA | B | 146 | 44.236 | 31.890 | 10.546 | 1.00 | 15.40 | C |
| ATOM | 3016 | O | ALA | B | 146 | 43.462 | 31.472 | 9.680 | 1.00 | 15.42 | O |
| ATOM | 3017 | CB | ALA | B | 146 | 43.000 | 33.459 | 12.076 | 1.00 | 15.51 | C |
| ATOM | 3018 | N | ARG | B | 147 | 45.525 | 32.147 | 10.318 | 1.00 | 15.24 | N |
| ATOM | 3019 | CA | ARG | B | 147 | 46.177 | 31.907 | 9.029 | 1.00 | 14.90 | C |
| ATOM | 3020 | C | ARG | B | 147 | 46.432 | 30.416 | 8.801 | 1.00 | 15.02 | C |
| ATOM | 3021 | O | ARG | B | 147 | 46.545 | 29.968 | 7.661 | 1.00 | 15.05 | O |
| ATOM | 3022 | CB | ARG | B | 147 | 47.492 | 32.695 | 8.934 | 1.00 | 14.62 | C |
| ATOM | 3023 | CG | ARG | B | 147 | 48.573 | 32.241 | 9.913 | 1.00 | 14.24 | C |
| ATOM | 3024 | CD | ARG | B | 147 | 49.880 | 33.010 | 9.835 | 1.00 | 13.92 | C |
| ATOM | 3025 | NE | ARG | B | 147 | 50.873 | 32.464 | 10.760 | 1.00 | 13.72 | N |
| ATOM | 3026 | CZ | ARG | B | 147 | 51.056 | 32.881 | 12.011 | 1.00 | 13.74 | C |
| ATOM | 3027 | NH1 | ARG | B | 147 | 50.318 | 33.865 | 12.511 | 1.00 | 13.22 | N |
| ATOM | 3028 | NH2 | ARG | B | 147 | 51.981 | 32.308 | 12.771 | 1.00 | 13.81 | N |
| ATOM | 3029 | N | ASN | B | 148 | 46.533 | 29.662 | 9.895 | 1.00 | 15.09 | N |
| ATOM | 3030 | CA | ASN | B | 148 | 46.710 | 28.214 | 9.840 | 1.00 | 15.09 | C |
| ATOM | 3031 | C | ASN | B | 148 | 45.393 | 27.473 | 10.078 | 1.00 | 15.13 | C |
| ATOM | 3032 | O | ASN | B | 148 | 45.367 | 26.387 | 10.662 | 1.00 | 15.07 | O |
| ATOM | 3033 | CB | ASN | B | 148 | 47.792 | 27.757 | 10.829 | 1.00 | 15.10 | C |
| ATOM | 3034 | CG | ASN | B | 148 | 49.191 | 28.191 | 10.412 | 1.00 | 15.28 | C |
| ATOM | 3035 | OD1 | ASN | B | 148 | 49.506 | 28.264 | 9.226 | 1.00 | 15.25 | O |
| ATOM | 3036 | ND2 | ASN | B | 148 | 50.037 | 28.480 | 11.392 | 1.00 | 15.40 | N |
| ATOM | 3037 | N | VAL | B | 149 | 44.299 | 28.086 | 9.630 | 1.00 | 15.20 | N |
| ATOM | 3038 | CA | VAL | B | 149 | 42.990 | 27.444 | 9.608 | 1.00 | 15.33 | C |
| ATOM | 3039 | C | VAL | B | 149 | 42.419 | 27.600 | 8.202 | 1.00 | 15.55 | C |
| ATOM | 3040 | O | VAL | B | 149 | 42.070 | 28.708 | 7.785 | 1.00 | 15.74 | O |
| ATOM | 3041 | CB | VAL | B | 149 | 42.015 | 28.047 | 10.651 | 1.00 | 15.25 | C |
| ATOM | 3042 | CG1 | VAL | B | 149 | 40.663 | 27.350 | 10.589 | 1.00 | 14.94 | C |
| ATOM | 3043 | CG2 | VAL | B | 149 | 42.593 | 27.957 | 12.060 | 1.00 | 15.54 | C |
| ATOM | 3044 | N | LEU | B | 150 | 42.334 | 26.489 | 7.475 | 1.00 | 15.45 | N |
| ATOM | 3045 | CA | LEU | B | 150 | 41.876 | 26.511 | 6.089 | 1.00 | 15.54 | C |
| ATOM | 3046 | C | LEU | B | 150 | 40.356 | 26.391 | 5.953 | 1.00 | 15.55 | C |
| ATOM | 3047 | O | LEU | B | 150 | 39.698 | 25.756 | 6.780 | 1.00 | 15.45 | O |
| ATOM | 3048 | CB | LEU | B | 150 | 42.583 | 25.429 | 5.270 | 1.00 | 15.58 | C |
| ATOM | 3049 | CG | LEU | B | 150 | 44.086 | 25.620 | 5.036 | 1.00 | 15.49 | C |
| ATOM | 3050 | CD1 | LEU | B | 150 | 44.684 | 24.382 | 4.380 | 1.00 | 15.15 | C |
| ATOM | 3051 | CD2 | LEU | B | 150 | 44.382 | 26.874 | 4.210 | 1.00 | 15.40 | C |
| ATOM | 3052 | N | VAL | B | 151 | 39.819 | 27.005 | 4.901 | 1.00 | 15.39 | N |
| ATOM | 3053 | CA | VAL | B | 151 | 38.388 | 26.986 | 4.613 | 1.00 | 15.29 | C |
| ATOM | 3054 | C | VAL | B | 151 | 38.078 | 25.907 | 3.577 | 1.00 | 15.56 | C |
| ATOM | 3055 | O | VAL | B | 151 | 38.458 | 26.034 | 2.409 | 1.00 | 15.39 | O |

FIG. 4YY

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3056 | CB | VAL | B | 151 | 37.894 | 28.371 | 4.095 | 1.00 | 15.34 | C |
| ATOM | 3057 | CG1 | VAL | B | 151 | 36.407 | 28.339 | 3.753 | 1.00 | 15.08 | C |
| ATOM | 3058 | CG2 | VAL | B | 151 | 38.183 | 29.474 | 5.110 | 1.00 | 14.95 | C |
| ATOM | 3059 | N | LYS | B | 152 | 37.406 | 24.841 | 4.010 | 1.00 | 15.80 | N |
| ATOM | 3060 | CA | LYS | B | 152 | 36.938 | 23.803 | 3.093 | 1.00 | 16.19 | C |
| ATOM | 3061 | C | LYS | B | 152 | 35.669 | 24.294 | 2.406 | 1.00 | 16.30 | C |
| ATOM | 3062 | O | LYS | B | 152 | 35.595 | 24.343 | 1.175 | 1.00 | 16.40 | O |
| ATOM | 3063 | CB | LYS | B | 152 | 36.690 | 22.482 | 3.828 | 1.00 | 16.33 | C |
| ATOM | 3064 | CG | LYS | B | 152 | 36.565 | 21.273 | 2.907 | 1.00 | 16.80 | C |
| ATOM | 3065 | CD | LYS | B | 152 | 36.069 | 20.045 | 3.657 | 1.00 | 17.29 | C |
| ATOM | 3066 | CE | LYS | B | 152 | 35.664 | 18.933 | 2.696 | 1.00 | 17.47 | C |
| ATOM | 3067 | NZ | LYS | B | 152 | 36.842 | 18.180 | 2.180 | 1.00 | 18.15 | N |
| ATOM | 3068 | N | THR | B | 153 | 34.673 | 24.635 | 3.219 | 1.00 | 16.35 | N |
| ATOM | 3069 | CA | THR | B | 153 | 33.512 | 25.412 | 2.794 | 1.00 | 16.56 | C |
| ATOM | 3070 | C | THR | B | 153 | 33.318 | 26.491 | 3.862 | 1.00 | 16.47 | C |
| ATOM | 3071 | O | THR | B | 153 | 33.941 | 26.409 | 4.922 | 1.00 | 16.60 | O |
| ATOM | 3072 | CB | THR | B | 153 | 32.244 | 24.528 | 2.683 | 1.00 | 16.59 | C |
| ATOM | 3073 | OG1 | THR | B | 153 | 31.869 | 24.054 | 3.981 | 1.00 | 17.12 | O |
| ATOM | 3074 | CG2 | THR | B | 153 | 32.510 | 23.250 | 1.893 | 1.00 | 16.76 | C |
| ATOM | 3075 | N | PRO | B | 154 | 32.487 | 27.503 | 3.606 | 1.00 | 16.43 | N |
| ATOM | 3076 | CA | PRO | B | 154 | 32.172 | 28.503 | 4.637 | 1.00 | 16.36 | C |
| ATOM | 3077 | C | PRO | B | 154 | 31.725 | 27.882 | 5.967 | 1.00 | 16.32 | C |
| ATOM | 3078 | O | PRO | B | 154 | 31.873 | 28.517 | 7.013 | 1.00 | 16.22 | O |
| ATOM | 3079 | CB | PRO | B | 154 | 31.027 | 29.300 | 4.008 | 1.00 | 16.41 | C |
| ATOM | 3080 | CG | PRO | B | 154 | 31.269 | 29.196 | 2.547 | 1.00 | 16.53 | C |
| ATOM | 3081 | CD | PRO | B | 154 | 31.818 | 27.810 | 2.326 | 1.00 | 16.53 | C |
| ATOM | 3082 | N | GLN | B | 155 | 31.210 | 26.653 | 5.918 | 1.00 | 16.31 | N |
| ATOM | 3083 | CA | GLN | B | 155 | 30.746 | 25.946 | 7.113 | 1.00 | 16.12 | C |
| ATOM | 3084 | C | GLN | B | 155 | 31.713 | 24.868 | 7.614 | 1.00 | 15.78 | C |
| ATOM | 3085 | O | GLN | B | 155 | 31.458 | 24.234 | 8.638 | 1.00 | 15.82 | O |
| ATOM | 3086 | CB | GLN | B | 155 | 29.348 | 25.345 | 6.891 | 1.00 | 16.33 | C |
| ATOM | 3087 | CG | GLN | B | 155 | 28.877 | 25.304 | 5.442 | 1.00 | 16.87 | C |
| ATOM | 3088 | CD | GLN | B | 155 | 27.835 | 26.364 | 5.132 | 1.00 | 17.45 | C |
| ATOM | 3089 | OE1 | GLN | B | 155 | 27.972 | 27.115 | 4.159 | 1.00 | 17.28 | O |
| ATOM | 3090 | NE2 | GLN | B | 155 | 26.791 | 26.430 | 5.955 | 1.00 | 17.68 | N |
| ATOM | 3091 | N | HIS | B | 156 | 32.819 | 24.669 | 6.902 | 1.00 | 15.45 | N |
| ATOM | 3092 | CA | HIS | B | 156 | 33.798 | 23.642 | 7.261 | 1.00 | 15.21 | C |
| ATOM | 3093 | C | HIS | B | 156 | 35.227 | 24.191 | 7.244 | 1.00 | 15.03 | C |
| ATOM | 3094 | O | HIS | B | 156 | 35.750 | 24.551 | 6.191 | 1.00 | 14.92 | O |
| ATOM | 3095 | CB | HIS | B | 156 | 33.668 | 22.435 | 6.319 | 1.00 | 15.13 | C |
| ATOM | 3096 | CG | HIS | B | 156 | 34.241 | 21.160 | 6.865 | 1.00 | 14.83 | C |
| ATOM | 3097 | ND1 | HIS | B | 156 | 33.918 | 19.924 | 6.348 | 1.00 | 14.44 | N |
| ATOM | 3098 | CE1 | HIS | B | 156 | 34.569 | 18.986 | 7.011 | 1.00 | 13.87 | C |
| ATOM | 3099 | NE2 | HIS | B | 156 | 35.303 | 19.569 | 7.942 | 1.00 | 13.92 | N |
| ATOM | 3100 | CD2 | HIS | B | 156 | 35.119 | 20.928 | 7.870 | 1.00 | 14.33 | C |
| ATOM | 3101 | N | VAL | B | 157 | 35.851 | 24.254 | 8.418 | 1.00 | 14.99 | N |
| ATOM | 3102 | CA | VAL | B | 157 | 37.221 | 24.757 | 8.540 | 1.00 | 14.97 | C |
| ATOM | 3103 | C | VAL | B | 157 | 38.180 | 23.715 | 9.130 | 1.00 | 15.29 | C |
| ATOM | 3104 | O | VAL | B | 157 | 37.805 | 22.945 | 10.018 | 1.00 | 15.40 | O |
| ATOM | 3105 | CB | VAL | B | 157 | 37.298 | 26.090 | 9.336 | 1.00 | 14.72 | C |
| ATOM | 3106 | CG1 | VAL | B | 157 | 36.646 | 27.225 | 8.556 | 1.00 | 14.48 | C |
| ATOM | 3107 | CG2 | VAL | B | 157 | 36.676 | 25.954 | 10.720 | 1.00 | 14.77 | C |
| ATOM | 3108 | N | LYS | B | 158 | 39.413 | 23.696 | 8.623 | 1.00 | 15.44 | N |
| ATOM | 3109 | CA | LYS | B | 158 | 40.409 | 22.708 | 9.036 | 1.00 | 15.73 | C |
| ATOM | 3110 | C | LYS | B | 158 | 41.712 | 23.358 | 9.501 | 1.00 | 15.85 | C |
| ATOM | 3111 | O | LYS | B | 158 | 42.260 | 24.231 | 8.823 | 1.00 | 15.82 | O |
| ATOM | 3112 | CB | LYS | B | 158 | 40.716 | 21.734 | 7.893 | 1.00 | 15.69 | C |
| ATOM | 3113 | CG | LYS | B | 158 | 39.558 | 20.858 | 7.450 | 1.00 | 16.28 | C |
| ATOM | 3114 | CD | LYS | B | 158 | 39.857 | 20.192 | 6.117 | 1.00 | 16.25 | C |
| ATOM | 3115 | CE | LYS | B | 158 | 39.785 | 18.673 | 6.225 | 1.00 | 16.82 | C |

FIG. 4ZZ

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3116 | NZ | LYS | B | 158 | 41.043 | 18.074 | 6.764 | 1.00 | 16.59 | N |
| ATOM | 3117 | N | ILE | B | 159 | 42.201 | 22.922 | 10.658 | 1.00 | 15.85 | N |
| ATOM | 3118 | CA | ILE | B | 159 | 43.514 | 23.332 | 11.143 | 1.00 | 15.88 | C |
| ATOM | 3119 | C | ILE | B | 159 | 44.590 | 22.696 | 10.264 | 1.00 | 16.08 | C |
| ATOM | 3120 | O | ILE | B | 159 | 44.486 | 21.524 | 9.889 | 1.00 | 15.98 | O |
| ATOM | 3121 | CB | ILE | B | 159 | 43.705 | 22.932 | 12.626 | 1.00 | 15.81 | C |
| ATOM | 3122 | CG1 | ILE | B | 159 | 42.600 | 23.536 | 13.497 | 1.00 | 15.59 | C |
| ATOM | 3123 | CD1 | ILE | B | 159 | 42.316 | 22.751 | 14.754 | 1.00 | 15.22 | C |
| ATOM | 3124 | CG2 | ILE | B | 159 | 45.077 | 23.369 | 13.135 | 1.00 | 15.73 | C |
| ATOM | 3125 | N | THR | B | 160 | 45.611 | 23.483 | 9.932 | 1.00 | 16.19 | N |
| ATOM | 3126 | CA | THR | B | 160 | 46.715 | 23.028 | 9.089 | 1.00 | 16.39 | C |
| ATOM | 3127 | C | THR | B | 160 | 48.058 | 23.378 | 9.727 | 1.00 | 16.67 | C |
| ATOM | 3128 | O | THR | B | 160 | 48.105 | 24.116 | 10.711 | 1.00 | 16.53 | O |
| ATOM | 3129 | CB | THR | B | 160 | 46.596 | 23.631 | 7.661 | 1.00 | 16.35 | C |
| ATOM | 3130 | OG1 | THR | B | 160 | 47.731 | 23.248 | 6.870 | 1.00 | 16.23 | O |
| ATOM | 3131 | CG2 | THR | B | 160 | 46.683 | 25.156 | 7.695 | 1.00 | 15.94 | C |
| ATOM | 3132 | N | ASP | B | 161 | 49.137 | 22.839 | 9.159 | 1.00 | 17.21 | N |
| ATOM | 3133 | CA | ASP | B | 161 | 50.513 | 23.080 | 9.621 | 1.00 | 17.93 | C |
| ATOM | 3134 | C | ASP | B | 161 | 50.819 | 22.527 | 11.015 | 1.00 | 18.47 | C |
| ATOM | 3135 | O | ASP | B | 161 | 51.803 | 22.925 | 11.647 | 1.00 | 18.68 | O |
| ATOM | 3136 | CB | ASP | B | 161 | 50.871 | 24.572 | 9.555 | 1.00 | 17.73 | C |
| ATOM | 3137 | CG | ASP | B | 161 | 51.033 | 25.074 | 8.138 | 1.00 | 17.77 | C |
| ATOM | 3138 | OD1 | ASP | B | 161 | 51.278 | 24.259 | 7.227 | 1.00 | 17.71 | O |
| ATOM | 3139 | OD2 | ASP | B | 161 | 50.933 | 26.279 | 7.837 | 1.00 | 18.29 | O |
| ATOM | 3140 | N | PHE | B | 162 | 49.977 | 21.613 | 11.487 | 1.00 | 19.04 | N |
| ATOM | 3141 | CA | PHE | B | 162 | 50.176 | 20.972 | 12.783 | 1.00 | 19.68 | C |
| ATOM | 3142 | C | PHE | B | 162 | 51.543 | 20.292 | 12.833 | 1.00 | 20.09 | C |
| ATOM | 3143 | O | PHE | B | 162 | 51.934 | 19.592 | 11.891 | 1.00 | 20.13 | O |
| ATOM | 3144 | CB | PHE | B | 162 | 49.052 | 19.965 | 13.065 | 1.00 | 19.79 | C |
| ATOM | 3145 | CG | PHE | B | 162 | 49.025 | 18.803 | 12.115 | 1.00 | 19.88 | C |
| ATOM | 3146 | CD1 | PHE | B | 162 | 49.475 | 17.556 | 12.518 | 1.00 | 20.15 | C |
| ATOM | 3147 | CE1 | PHE | B | 162 | 49.459 | 16.479 | 11.636 | 1.00 | 20.74 | C |
| ATOM | 3148 | CZ | PHE | B | 162 | 48.990 | 16.645 | 10.336 | 1.00 | 20.08 | C |
| ATOM | 3149 | CE2 | PHE | B | 162 | 48.548 | 17.887 | 9.923 | 1.00 | 20.37 | C |
| ATOM | 3150 | CD2 | PHE | B | 162 | 48.559 | 18.958 | 10.811 | 1.00 | 20.47 | C |
| ATOM | 3151 | N | GLY | B | 163 | 52.271 | 20.527 | 13.925 | 1.00 | 20.48 | N |
| ATOM | 3152 | CA | GLY | B | 163 | 53.586 | 19.945 | 14.129 | 1.00 | 20.74 | C |
| ATOM | 3153 | C | GLY | B | 163 | 54.492 | 20.057 | 12.916 | 1.00 | 21.18 | C |
| ATOM | 3154 | O | GLY | B | 163 | 54.865 | 19.045 | 12.322 | 1.00 | 21.69 | O |
| ATOM | 3155 | N | LEU | B | 164 | 54.815 | 21.291 | 12.536 | 1.00 | 21.26 | N |
| ATOM | 3156 | CA | LEU | B | 164 | 55.793 | 21.569 | 11.487 | 1.00 | 21.32 | C |
| ATOM | 3157 | C | LEU | B | 164 | 57.021 | 22.244 | 12.091 | 1.00 | 21.56 | C |
| ATOM | 3158 | O | LEU | B | 164 | 58.064 | 22.361 | 11.442 | 1.00 | 21.57 | O |
| ATOM | 3159 | CB | LEU | B | 164 | 55.200 | 22.490 | 10.417 | 1.00 | 21.23 | C |
| ATOM | 3160 | CG | LEU | B | 164 | 54.224 | 21.977 | 9.354 | 1.00 | 21.46 | C |
| ATOM | 3161 | CD1 | LEU | B | 164 | 54.060 | 23.039 | 8.293 | 1.00 | 21.29 | C |
| ATOM | 3162 | CD2 | LEU | B | 164 | 54.690 | 20.689 | 8.712 | 1.00 | 21.59 | C |
| ATOM | 3163 | N | ALA | B | 165 | 56.886 | 22.691 | 13.338 | 1.00 | 21.73 | N |
| ATOM | 3164 | CA | ALA | B | 165 | 57.956 | 23.396 | 14.035 | 1.00 | 21.74 | C |
| ATOM | 3165 | C | ALA | B | 165 | 59.047 | 22.447 | 14.528 | 1.00 | 21.84 | C |
| ATOM | 3166 | O | ALA | B | 165 | 60.149 | 22.886 | 14.868 | 1.00 | 22.15 | O |
| ATOM | 3167 | CB | ALA | B | 165 | 57.390 | 24.216 | 15.183 | 1.00 | 21.73 | C |
| ATOM | 3168 | N | LYS | B | 166 | 58.732 | 21.153 | 14.567 | 1.00 | 21.83 | N |
| ATOM | 3169 | CA | LYS | B | 166 | 59.709 | 20.115 | 14.891 | 1.00 | 21.68 | C |
| ATOM | 3170 | C | LYS | B | 166 | 60.661 | 19.920 | 13.715 | 1.00 | 21.83 | C |
| ATOM | 3171 | O | LYS | B | 166 | 60.234 | 19.879 | 12.554 | 1.00 | 22.08 | O |
| ATOM | 3172 | CB | LYS | B | 166 | 59.011 | 18.789 | 15.214 | 1.00 | 21.77 | C |
| ATOM | 3173 | CG | LYS | B | 166 | 58.011 | 18.840 | 16.373 | 1.00 | 21.98 | C |
| ATOM | 3174 | CD | LYS | B | 166 | 57.480 | 17.442 | 16.695 | 1.00 | 22.41 | C |
| ATOM | 3175 | CE | LYS | B | 166 | 56.098 | 17.498 | 17.346 | 1.00 | 22.83 | C |

FIG. 4AAA

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3176 | NZ | LYS | B | 166 | 55.809 | 16.260 | 18.145 | 1.00 | 22.79 | N |
| ATOM | 3177 | N | PRO | B | 183 | 56.715 | 33.625 | 15.625 | 1.00 | 22.42 | N |
| ATOM | 3178 | CA | PRO | B | 183 | 55.580 | 34.544 | 15.765 | 1.00 | 22.25 | C |
| ATOM | 3179 | C | PRO | B | 183 | 55.212 | 34.748 | 17.232 | 1.00 | 22.18 | C |
| ATOM | 3180 | O | PRO | B | 183 | 54.353 | 34.045 | 17.774 | 1.00 | 22.27 | O |
| ATOM | 3181 | CB | PRO | B | 183 | 54.457 | 33.829 | 15.009 | 1.00 | 22.31 | C |
| ATOM | 3182 | CG | PRO | B | 183 | 55.172 | 32.930 | 14.053 | 1.00 | 22.53 | C |
| ATOM | 3183 | CD | PRO | B | 183 | 56.379 | 32.450 | 14.804 | 1.00 | 22.50 | C |
| ATOM | 3184 | N | ILE | B | 184 | 55.881 | 35.719 | 17.851 | 1.00 | 21.96 | N |
| ATOM | 3185 | CA | ILE | B | 184 | 55.735 | 36.052 | 19.267 | 1.00 | 21.71 | C |
| ATOM | 3186 | C | ILE | B | 184 | 54.295 | 36.406 | 19.654 | 1.00 | 21.65 | C |
| ATOM | 3187 | O | ILE | B | 184 | 53.838 | 36.060 | 20.749 | 1.00 | 21.87 | O |
| ATOM | 3188 | CB | ILE | B | 184 | 56.713 | 37.217 | 19.626 | 1.00 | 21.83 | C |
| ATOM | 3189 | CG1 | ILE | B | 184 | 58.176 | 36.777 | 19.453 | 1.00 | 21.78 | C |
| ATOM | 3190 | CD1 | ILE | B | 184 | 58.720 | 35.862 | 20.554 | 1.00 | 22.06 | C |
| ATOM | 3191 | CG2 | ILE | B | 184 | 56.444 | 37.788 | 21.028 | 1.00 | 21.83 | C |
| ATOM | 3192 | N | LYS | B | 185 | 53.585 | 37.074 | 18.747 | 1.00 | 21.28 | N |
| ATOM | 3193 | CA | LYS | B | 185 | 52.247 | 37.607 | 19.024 | 1.00 | 20.93 | C |
| ATOM | 3194 | C | LYS | B | 185 | 51.169 | 36.536 | 19.241 | 1.00 | 20.79 | C |
| ATOM | 3195 | O | LYS | B | 185 | 50.058 | 36.849 | 19.677 | 1.00 | 20.47 | O |
| ATOM | 3196 | CB | LYS | B | 185 | 51.823 | 38.590 | 17.926 | 1.00 | 20.75 | C |
| ATOM | 3197 | CG | LYS | B | 185 | 52.863 | 39.659 | 17.628 | 1.00 | 20.34 | C |
| ATOM | 3198 | CD | LYS | B | 185 | 52.235 | 40.912 | 17.060 | 1.00 | 19.80 | C |
| ATOM | 3199 | CE | LYS | B | 185 | 52.892 | 42.156 | 17.628 | 1.00 | 19.51 | C |
| ATOM | 3200 | NZ | LYS | B | 185 | 53.140 | 43.181 | 16.583 | 1.00 | 19.03 | N |
| ATOM | 3201 | N | TRP | B | 186 | 51.510 | 35.282 | 18.950 | 1.00 | 20.74 | N |
| ATOM | 3202 | CA | TRP | B | 186 | 50.610 | 34.151 | 19.176 | 1.00 | 20.82 | C |
| ATOM | 3203 | C | TRP | B | 186 | 51.092 | 33.236 | 20.299 | 1.00 | 21.08 | C |
| ATOM | 3204 | O | TRP | B | 186 | 50.361 | 32.350 | 20.742 | 1.00 | 21.18 | O |
| ATOM | 3205 | CB | TRP | B | 186 | 50.440 | 33.341 | 17.890 | 1.00 | 20.63 | C |
| ATOM | 3206 | CG | TRP | B | 186 | 49.500 | 33.972 | 16.921 | 1.00 | 19.96 | C |
| ATOM | 3207 | CD1 | TRP | B | 186 | 48.182 | 33.667 | 16.742 | 1.00 | 19.61 | C |
| ATOM | 3208 | NE1 | TRP | B | 186 | 47.640 | 34.464 | 15.762 | 1.00 | 19.54 | N |
| ATOM | 3209 | CE2 | TRP | B | 186 | 48.612 | 35.306 | 15.285 | 1.00 | 19.48 | C |
| ATOM | 3210 | CD2 | TRP | B | 186 | 49.799 | 35.023 | 15.996 | 1.00 | 19.21 | C |
| ATOM | 3211 | CE3 | TRP | B | 186 | 50.954 | 35.757 | 15.690 | 1.00 | 18.81 | C |
| ATOM | 3212 | CZ3 | TRP | B | 186 | 50.888 | 36.737 | 14.700 | 1.00 | 18.50 | C |
| ATOM | 3213 | CH2 | TRP | B | 186 | 49.691 | 36.993 | 14.014 | 1.00 | 18.50 | C |
| ATOM | 3214 | CZ2 | TRP | B | 186 | 48.545 | 36.294 | 14.291 | 1.00 | 18.96 | C |
| ATOM | 3215 | N | MET | B | 187 | 52.319 | 33.467 | 20.760 | 1.00 | 21.43 | N |
| ATOM | 3216 | CA | MET | B | 187 | 52.975 | 32.579 | 21.715 | 1.00 | 21.61 | C |
| ATOM | 3217 | C | MET | B | 187 | 52.628 | 32.876 | 23.168 | 1.00 | 21.85 | C |
| ATOM | 3218 | O | MET | B | 187 | 52.400 | 34.030 | 23.545 | 1.00 | 21.99 | O |
| ATOM | 3219 | CB | MET | B | 187 | 54.492 | 32.637 | 21.536 | 1.00 | 21.62 | C |
| ATOM | 3220 | CG | MET | B | 187 | 55.005 | 31.890 | 20.320 | 1.00 | 21.92 | C |
| ATOM | 3221 | SD | MET | B | 187 | 56.599 | 32.519 | 19.779 | 1.00 | 23.04 | S |
| ATOM | 3222 | CE | MET | B | 187 | 57.688 | 31.747 | 20.961 | 1.00 | 22.66 | C |
| ATOM | 3223 | N | ALA | B | 188 | 52.596 | 31.818 | 23.976 | 1.00 | 21.96 | N |
| ATOM | 3224 | CA | ALA | B | 188 | 52.451 | 31.941 | 25.421 | 1.00 | 21.93 | C |
| ATOM | 3225 | C | ALA | B | 188 | 53.754 | 32.467 | 26.022 | 1.00 | 21.97 | C |
| ATOM | 3226 | O | ALA | B | 188 | 54.826 | 32.291 | 25.435 | 1.00 | 21.90 | O |
| ATOM | 3227 | CB | ALA | B | 188 | 52.082 | 30.600 | 26.026 | 1.00 | 21.97 | C |
| ATOM | 3228 | N | LEU | B | 189 | 53.657 | 33.106 | 27.188 | 1.00 | 21.93 | N |
| ATOM | 3229 | CA | LEU | B | 189 | 54.824 | 33.690 | 27.856 | 1.00 | 21.88 | C |
| ATOM | 3230 | C | LEU | B | 189 | 55.943 | 32.675 | 28.087 | 1.00 | 21.74 | C |
| ATOM | 3231 | O | LEU | B | 189 | 57.116 | 32.990 | 27.880 | 1.00 | 22.00 | O |
| ATOM | 3232 | CB | LEU | B | 189 | 54.426 | 34.362 | 29.176 | 1.00 | 22.00 | C |
| ATOM | 3233 | CG | LEU | B | 189 | 55.451 | 35.311 | 29.813 | 1.00 | 22.38 | C |
| ATOM | 3234 | CD1 | LEU | B | 189 | 55.537 | 36.650 | 29.084 | 1.00 | 22.36 | C |
| ATOM | 3235 | CD2 | LEU | B | 189 | 55.142 | 35.528 | 31.288 | 1.00 | 22.97 | C |

FIG. 4BBB

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3236 | N | GLU | B | 190 | 55.575 | 31.463 | 28.501 | 1.00 | 21.45 | N |
| ATOM | 3237 | CA | GLU | B | 190 | 56.541 | 30.386 | 28.726 | 1.00 | 21.15 | C |
| ATOM | 3238 | C | GLU | B | 190 | 57.252 | 29.959 | 27.439 | 1.00 | 21.17 | C |
| ATOM | 3239 | O | GLU | B | 190 | 58.408 | 29.532 | 27.475 | 1.00 | 21.19 | O |
| ATOM | 3240 | CB | GLU | B | 190 | 55.881 | 29.183 | 29.419 | 1.00 | 21.12 | C |
| ATOM | 3241 | CG | GLU | B | 190 | 54.757 | 28.513 | 28.640 | 1.00 | 20.85 | C |
| ATOM | 3242 | CD | GLU | B | 190 | 53.377 | 29.014 | 29.030 | 1.00 | 20.68 | C |
| ATOM | 3243 | OE1 | GLU | B | 190 | 52.434 | 28.197 | 29.037 | 1.00 | 20.64 | O |
| ATOM | 3244 | OE2 | GLU | B | 190 | 53.225 | 30.221 | 29.320 | 1.00 | 20.22 | O |
| ATOM | 3245 | N | SER | B | 191 | 56.559 | 30.086 | 26.309 | 1.00 | 21.18 | N |
| ATOM | 3246 | CA | SER | B | 191 | 57.142 | 29.788 | 25.003 | 1.00 | 21.15 | C |
| ATOM | 3247 | C | SER | B | 191 | 58.086 | 30.902 | 24.567 | 1.00 | 21.19 | C |
| ATOM | 3248 | O | SER | B | 191 | 59.075 | 30.653 | 23.880 | 1.00 | 21.13 | O |
| ATOM | 3249 | CB | SER | B | 191 | 56.048 | 29.582 | 23.953 | 1.00 | 21.15 | C |
| ATOM | 3250 | OG | SER | B | 191 | 55.160 | 28.546 | 24.330 | 1.00 | 20.81 | O |
| ATOM | 3251 | N | ILE | B | 192 | 57.774 | 32.132 | 24.969 | 1.00 | 21.42 | N |
| ATOM | 3252 | CA | ILE | B | 192 | 58.617 | 33.279 | 24.643 | 1.00 | 21.55 | C |
| ATOM | 3253 | C | ILE | B | 192 | 59.885 | 33.273 | 25.501 | 1.00 | 21.47 | C |
| ATOM | 3254 | O | ILE | B | 192 | 60.990 | 33.442 | 24.982 | 1.00 | 21.39 | O |
| ATOM | 3255 | CB | ILE | B | 192 | 57.832 | 34.613 | 24.791 | 1.00 | 21.56 | C |
| ATOM | 3256 | CG1 | ILE | B | 192 | 56.640 | 34.643 | 23.833 | 1.00 | 21.77 | C |
| ATOM | 3257 | CD1 | ILE | B | 192 | 55.467 | 35.476 | 24.324 | 1.00 | 22.48 | C |
| ATOM | 3258 | CG2 | ILE | B | 192 | 58.734 | 35.819 | 24.517 | 1.00 | 21.63 | C |
| ATOM | 3259 | N | LEU | B | 193 | 59.719 | 33.051 | 26.803 | 1.00 | 21.39 | N |
| ATOM | 3260 | CA | LEU | B | 193 | 60.829 | 33.146 | 27.750 | 1.00 | 21.60 | C |
| ATOM | 3261 | C | LEU | B | 193 | 61.710 | 31.902 | 27.789 | 1.00 | 21.76 | C |
| ATOM | 3262 | O | LEU | B | 193 | 62.937 | 32.012 | 27.864 | 1.00 | 21.97 | O |
| ATOM | 3263 | CB | LEU | B | 193 | 60.321 | 33.476 | 29.161 | 1.00 | 21.51 | C |
| ATOM | 3264 | CG | LEU | B | 193 | 59.616 | 34.819 | 29.392 | 1.00 | 21.65 | C |
| ATOM | 3265 | CD1 | LEU | B | 193 | 59.084 | 34.908 | 30.815 | 1.00 | 21.26 | C |
| ATOM | 3266 | CD2 | LEU | B | 193 | 60.528 | 36.005 | 29.083 | 1.00 | 21.67 | C |
| ATOM | 3267 | N | HIS | B | 194 | 61.087 | 30.726 | 27.736 | 1.00 | 21.75 | N |
| ATOM | 3268 | CA | HIS | B | 194 | 61.800 | 29.469 | 27.956 | 1.00 | 21.77 | C |
| ATOM | 3269 | C | HIS | B | 194 | 61.667 | 28.455 | 26.815 | 1.00 | 21.51 | C |
| ATOM | 3270 | O | HIS | B | 194 | 62.162 | 27.330 | 26.922 | 1.00 | 21.28 | O |
| ATOM | 3271 | CB | HIS | B | 194 | 61.348 | 28.839 | 29.278 | 1.00 | 22.22 | C |
| ATOM | 3272 | CG | HIS | B | 194 | 61.278 | 29.806 | 30.420 | 1.00 | 22.90 | C |
| ATOM | 3273 | ND1 | HIS | B | 194 | 62.286 | 30.703 | 30.701 | 1.00 | 23.67 | N |
| ATOM | 3274 | CE1 | HIS | B | 194 | 61.950 | 31.426 | 31.754 | 1.00 | 23.97 | C |
| ATOM | 3275 | NE2 | HIS | B | 194 | 60.760 | 31.028 | 32.169 | 1.00 | 24.36 | N |
| ATOM | 3276 | CD2 | HIS | B | 194 | 60.317 | 30.017 | 31.350 | 1.00 | 23.54 | C |
| ATOM | 3277 | N | ARG | B | 195 | 61.007 | 28.864 | 25.730 | 1.00 | 21.22 | N |
| ATOM | 3278 | CA | ARG | B | 195 | 60.785 | 28.018 | 24.547 | 1.00 | 20.95 | C |
| ATOM | 3279 | C | ARG | B | 195 | 60.075 | 26.692 | 24.863 | 1.00 | 20.83 | C |
| ATOM | 3280 | O | ARG | B | 195 | 60.388 | 25.652 | 24.270 | 1.00 | 20.76 | O |
| ATOM | 3281 | CB | ARG | B | 195 | 62.097 | 27.769 | 23.785 | 1.00 | 20.95 | C |
| ATOM | 3282 | CG | ARG | B | 195 | 62.869 | 29.026 | 23.414 | 1.00 | 20.97 | C |
| ATOM | 3283 | CD | ARG | B | 195 | 64.382 | 28.853 | 23.432 | 1.00 | 20.99 | C |
| ATOM | 3284 | N | ILE | B | 196 | 59.121 | 26.739 | 25.793 | 1.00 | 20.45 | N |
| ATOM | 3285 | CA | ILE | B | 196 | 58.351 | 25.559 | 26.183 | 1.00 | 20.11 | C |
| ATOM | 3286 | C | ILE | B | 196 | 56.993 | 25.551 | 25.484 | 1.00 | 19.80 | C |
| ATOM | 3287 | O | ILE | B | 196 | 56.243 | 26.527 | 25.540 | 1.00 | 19.93 | O |
| ATOM | 3288 | CB | ILE | B | 196 | 58.212 | 25.464 | 27.734 | 1.00 | 20.35 | C |
| ATOM | 3289 | CG1 | ILE | B | 196 | 59.547 | 25.040 | 28.363 | 1.00 | 20.33 | C |
| ATOM | 3290 | CD1 | ILE | B | 196 | 59.748 | 25.504 | 29.792 | 1.00 | 20.50 | C |
| ATOM | 3291 | CG2 | ILE | B | 196 | 57.118 | 24.463 | 28.136 | 1.00 | 20.41 | C |
| ATOM | 3292 | N | TYR | B | 197 | 56.695 | 24.442 | 24.814 | 1.00 | 19.45 | N |
| ATOM | 3293 | CA | TYR | B | 197 | 55.452 | 24.287 | 24.066 | 1.00 | 18.70 | C |
| ATOM | 3294 | C | TYR | B | 197 | 54.669 | 23.094 | 24.592 | 1.00 | 18.24 | C |
| ATOM | 3295 | O | TYR | B | 197 | 55.197 | 21.986 | 24.680 | 1.00 | 18.23 | O |

FIG. 4CCC

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3296 | CB | TYR | B | 197 | 55.747 | 24.098 | 22.574 | 1.00 | 18.72 | C |
| ATOM | 3297 | CG | TYR | B | 197 | 56.388 | 25.291 | 21.904 | 1.00 | 18.55 | C |
| ATOM | 3298 | CD1 | TYR | B | 197 | 55.616 | 26.225 | 21.216 | 1.00 | 18.24 | C |
| ATOM | 3299 | CE1 | TYR | B | 197 | 56.198 | 27.319 | 20.591 | 1.00 | 18.10 | C |
| ATOM | 3300 | CZ | TYR | B | 197 | 57.570 | 27.490 | 20.648 | 1.00 | 18.50 | C |
| ATOM | 3301 | OH | TYR | B | 197 | 58.148 | 28.575 | 20.030 | 1.00 | 19.03 | O |
| ATOM | 3302 | CE2 | TYR | B | 197 | 58.363 | 26.577 | 21.320 | 1.00 | 18.66 | C |
| ATOM | 3303 | CD2 | TYR | B | 197 | 57.770 | 25.480 | 21.942 | 1.00 | 18.69 | C |
| ATOM | 3304 | N | THR | B | 198 | 53.410 | 23.331 | 24.946 | 1.00 | 17.98 | N |
| ATOM | 3305 | CA | THR | B | 198 | 52.532 | 22.294 | 25.490 | 1.00 | 17.80 | C |
| ATOM | 3306 | C | THR | B | 198 | 51.153 | 22.399 | 24.855 | 1.00 | 17.59 | C |
| ATOM | 3307 | O | THR | B | 198 | 50.941 | 23.221 | 23.964 | 1.00 | 17.78 | O |
| ATOM | 3308 | CB | THR | B | 198 | 52.399 | 22.437 | 27.023 | 1.00 | 17.82 | C |
| ATOM | 3309 | OG1 | THR | B | 198 | 52.101 | 23.799 | 27.350 | 1.00 | 17.96 | O |
| ATOM | 3310 | CG2 | THR | B | 198 | 53.731 | 22.166 | 27.732 | 1.00 | 17.76 | C |
| ATOM | 3311 | N | HIS | B | 199 | 50.219 | 21.567 | 25.316 | 1.00 | 17.36 | N |
| ATOM | 3312 | CA | HIS | B | 199 | 48.819 | 21.664 | 24.906 | 1.00 | 17.22 | C |
| ATOM | 3313 | C | HIS | B | 199 | 48.213 | 22.963 | 25.426 | 1.00 | 17.24 | C |
| ATOM | 3314 | O | HIS | B | 199 | 47.380 | 23.575 | 24.758 | 1.00 | 16.92 | O |
| ATOM | 3315 | CB | HIS | B | 199 | 48.005 | 20.479 | 25.428 | 1.00 | 17.04 | C |
| ATOM | 3316 | CG | HIS | B | 199 | 48.575 | 19.143 | 25.067 | 1.00 | 16.91 | C |
| ATOM | 3317 | ND1 | HIS | B | 199 | 48.692 | 18.710 | 23.764 | 1.00 | 16.53 | N |
| ATOM | 3318 | CE1 | HIS | B | 199 | 49.220 | 17.499 | 23.751 | 1.00 | 16.36 | C |
| ATOM | 3319 | NE2 | HIS | B | 199 | 49.445 | 17.130 | 25.000 | 1.00 | 16.26 | N |
| ATOM | 3320 | CD2 | HIS | B | 199 | 49.050 | 18.140 | 25.842 | 1.00 | 16.15 | C |
| ATOM | 3321 | N | GLN | B | 200 | 48.646 | 23.366 | 26.622 | 1.00 | 17.27 | N |
| ATOM | 3322 | CA | GLN | B | 200 | 48.206 | 24.609 | 27.256 | 1.00 | 17.28 | C |
| ATOM | 3323 | C | GLN | B | 200 | 48.854 | 25.854 | 26.646 | 1.00 | 17.15 | C |
| ATOM | 3324 | O | GLN | B | 200 | 48.337 | 26.961 | 26.793 | 1.00 | 17.20 | O |
| ATOM | 3325 | CB | GLN | B | 200 | 48.452 | 24.558 | 28.766 | 1.00 | 17.38 | C |
| ATOM | 3326 | CG | GLN | B | 200 | 47.551 | 23.572 | 29.509 | 1.00 | 17.51 | C |
| ATOM | 3327 | CD | GLN | B | 200 | 46.077 | 23.760 | 29.184 | 1.00 | 17.43 | C |
| ATOM | 3328 | OE1 | GLN | B | 200 | 45.513 | 23.019 | 28.373 | 1.00 | 16.85 | O |
| ATOM | 3329 | NE2 | GLN | B | 200 | 45.453 | 24.750 | 29.814 | 1.00 | 17.27 | N |
| ATOM | 3330 | N | SER | B | 201 | 49.984 | 25.666 | 25.970 | 1.00 | 17.06 | N |
| ATOM | 3331 | CA | SER | B | 201 | 50.580 | 26.722 | 25.156 | 1.00 | 17.03 | C |
| ATOM | 3332 | C | SER | B | 201 | 49.790 | 26.896 | 23.859 | 1.00 | 16.80 | C |
| ATOM | 3333 | O | SER | B | 201 | 49.717 | 27.998 | 23.313 | 1.00 | 16.57 | O |
| ATOM | 3334 | CB | SER | B | 201 | 52.042 | 26.408 | 24.842 | 1.00 | 17.04 | C |
| ATOM | 3335 | OG | SER | B | 201 | 52.670 | 27.514 | 24.215 | 1.00 | 17.75 | O |
| ATOM | 3336 | N | ASP | B | 202 | 49.207 | 25.799 | 23.376 | 1.00 | 16.59 | N |
| ATOM | 3337 | CA | ASP | B | 202 | 48.321 | 25.820 | 22.215 | 1.00 | 16.53 | C |
| ATOM | 3338 | C | ASP | B | 202 | 46.986 | 26.495 | 22.535 | 1.00 | 16.38 | C |
| ATOM | 3339 | O | ASP | B | 202 | 46.330 | 27.026 | 21.636 | 1.00 | 16.51 | O |
| ATOM | 3340 | CB | ASP | B | 202 | 48.066 | 24.399 | 21.698 | 1.00 | 16.49 | C |
| ATOM | 3341 | CG | ASP | B | 202 | 49.124 | 23.924 | 20.714 | 1.00 | 16.64 | C |
| ATOM | 3342 | OD1 | ASP | B | 202 | 49.210 | 22.693 | 20.496 | 1.00 | 16.58 | O |
| ATOM | 3343 | OD2 | ASP | B | 202 | 49.906 | 24.693 | 20.108 | 1.00 | 16.43 | O |
| ATOM | 3344 | N | VAL | B | 203 | 46.585 | 26.461 | 23.807 | 1.00 | 16.20 | N |
| ATOM | 3345 | CA | VAL | B | 203 | 45.360 | 27.131 | 24.255 | 1.00 | 16.45 | C |
| ATOM | 3346 | C | VAL | B | 203 | 45.518 | 28.652 | 24.153 | 1.00 | 16.45 | C |
| ATOM | 3347 | O | VAL | B | 203 | 44.583 | 29.352 | 23.766 | 1.00 | 16.60 | O |
| ATOM | 3348 | CB | VAL | B | 203 | 44.933 | 26.712 | 25.699 | 1.00 | 16.39 | C |
| ATOM | 3349 | CG1 | VAL | B | 203 | 43.676 | 27.451 | 26.136 | 1.00 | 16.30 | C |
| ATOM | 3350 | CG2 | VAL | B | 203 | 44.685 | 25.209 | 25.786 | 1.00 | 16.35 | C |
| ATOM | 3351 | N | TRP | B | 204 | 46.708 | 29.147 | 24.491 | 1.00 | 16.36 | N |
| ATOM | 3352 | CA | TRP | B | 204 | 47.040 | 30.561 | 24.347 | 1.00 | 16.46 | C |
| ATOM | 3353 | C | TRP | B | 204 | 46.851 | 31.022 | 22.903 | 1.00 | 16.47 | C |
| ATOM | 3354 | O | TRP | B | 204 | 46.183 | 32.030 | 22.652 | 1.00 | 16.51 | O |
| ATOM | 3355 | CB | TRP | B | 204 | 48.479 | 30.821 | 24.799 | 1.00 | 16.57 | C |

FIG. 4DDD

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3356 | CG | TRP | B | 204 | 48.858 | 32.281 | 24.865 | 1.00 | 16.80 | C |
| ATOM | 3357 | CD1 | TRP | B | 204 | 48.956 | 33.158 | 23.817 | 1.00 | 16.53 | C |
| ATOM | 3358 | NE1 | TRP | B | 204 | 49.332 | 34.400 | 24.270 | 1.00 | 16.41 | N |
| ATOM | 3359 | CE2 | TRP | B | 204 | 49.492 | 34.350 | 25.629 | 1.00 | 16.34 | C |
| ATOM | 3360 | CD2 | TRP | B | 204 | 49.200 | 33.028 | 26.040 | 1.00 | 16.56 | C |
| ATOM | 3361 | CE3 | TRP | B | 204 | 49.294 | 32.714 | 27.402 | 1.00 | 16.37 | C |
| ATOM | 3362 | CZ3 | TRP | B | 204 | 49.669 | 33.717 | 28.299 | 1.00 | 16.86 | C |
| ATOM | 3363 | CH2 | TRP | B | 204 | 49.948 | 35.021 | 27.855 | 1.00 | 16.31 | C |
| ATOM | 3364 | CZ2 | TRP | B | 204 | 49.865 | 35.355 | 26.528 | 1.00 | 16.24 | C |
| ATOM | 3365 | N | SER | B | 205 | 47.438 | 30.275 | 21.965 | 1.00 | 16.22 | N |
| ATOM | 3366 | CA | SER | B | 205 | 47.342 | 30.578 | 20.534 | 1.00 | 15.80 | C |
| ATOM | 3367 | C | SER | B | 205 | 45.903 | 30.507 | 20.035 | 1.00 | 15.55 | C |
| ATOM | 3368 | O | SER | B | 205 | 45.511 | 31.285 | 19.165 | 1.00 | 15.61 | O |
| ATOM | 3369 | CB | SER | B | 205 | 48.224 | 29.635 | 19.714 | 1.00 | 15.70 | C |
| ATOM | 3370 | OG | SER | B | 205 | 49.559 | 29.641 | 20.181 | 1.00 | 15.55 | O |
| ATOM | 3371 | N | TYR | B | 206 | 45.129 | 29.571 | 20.588 | 1.00 | 15.07 | N |
| ATOM | 3372 | CA | TYR | B | 206 | 43.699 | 29.467 | 20.309 | 1.00 | 14.61 | C |
| ATOM | 3373 | C | TYR | B | 206 | 42.976 | 30.733 | 20.767 | 1.00 | 14.76 | C |
| ATOM | 3374 | O | TYR | B | 206 | 42.007 | 31.159 | 20.143 | 1.00 | 15.07 | O |
| ATOM | 3375 | CB | TYR | B | 206 | 43.105 | 28.223 | 20.986 | 1.00 | 14.35 | C |
| ATOM | 3376 | CG | TYR | B | 206 | 41.600 | 28.072 | 20.835 | 1.00 | 13.49 | C |
| ATOM | 3377 | CD1 | TYR | B | 206 | 40.733 | 28.424 | 21.871 | 1.00 | 12.79 | C |
| ATOM | 3378 | CE1 | TYR | B | 206 | 39.348 | 28.288 | 21.734 | 1.00 | 12.20 | C |
| ATOM | 3379 | CZ | TYR | B | 206 | 38.825 | 27.794 | 20.550 | 1.00 | 11.90 | C |
| ATOM | 3380 | OH | TYR | B | 206 | 37.467 | 27.651 | 20.399 | 1.00 | 10.89 | O |
| ATOM | 3381 | CE2 | TYR | B | 206 | 39.665 | 27.435 | 19.512 | 1.00 | 12.25 | C |
| ATOM | 3382 | CD2 | TYR | B | 206 | 41.045 | 27.574 | 19.659 | 1.00 | 12.84 | C |
| ATOM | 3383 | N | GLY | B | 207 | 43.456 | 31.330 | 21.856 | 1.00 | 14.75 | N |
| ATOM | 3384 | CA | GLY | B | 207 | 42.922 | 32.587 | 22.347 | 1.00 | 15.01 | C |
| ATOM | 3385 | C | GLY | B | 207 | 43.105 | 33.715 | 21.347 | 1.00 | 15.01 | C |
| ATOM | 3386 | O | GLY | B | 207 | 42.144 | 34.405 | 20.999 | 1.00 | 15.06 | O |
| ATOM | 3387 | N | VAL | B | 208 | 44.339 | 33.891 | 20.882 | 1.00 | 15.03 | N |
| ATOM | 3388 | CA | VAL | B | 208 | 44.664 | 34.892 | 19.864 | 1.00 | 15.14 | C |
| ATOM | 3389 | C | VAL | B | 208 | 43.905 | 34.632 | 18.559 | 1.00 | 15.22 | C |
| ATOM | 3390 | O | VAL | B | 208 | 43.474 | 35.574 | 17.893 | 1.00 | 15.27 | O |
| ATOM | 3391 | CB | VAL | B | 208 | 46.189 | 34.962 | 19.593 | 1.00 | 15.17 | C |
| ATOM | 3392 | CG1 | VAL | B | 208 | 46.527 | 36.111 | 18.649 | 1.00 | 15.05 | C |
| ATOM | 3393 | CG2 | VAL | B | 208 | 46.965 | 35.102 | 20.903 | 1.00 | 15.18 | C |
| ATOM | 3394 | N | THR | B | 209 | 43.734 | 33.353 | 18.220 | 1.00 | 15.32 | N |
| ATOM | 3395 | CA | THR | B | 209 | 43.005 | 32.934 | 17.020 | 1.00 | 15.51 | C |
| ATOM | 3396 | C | THR | B | 209 | 41.534 | 33.362 | 17.054 | 1.00 | 15.77 | C |
| ATOM | 3397 | O | THR | B | 209 | 41.041 | 33.969 | 16.100 | 1.00 | 15.74 | O |
| ATOM | 3398 | CB | THR | B | 209 | 43.125 | 31.405 | 16.820 | 1.00 | 15.39 | C |
| ATOM | 3399 | OG1 | THR | B | 209 | 44.509 | 31.045 | 16.726 | 1.00 | 15.35 | O |
| ATOM | 3400 | CG2 | THR | B | 209 | 42.566 | 30.986 | 15.468 | 1.00 | 15.10 | C |
| ATOM | 3401 | N | VAL | B | 210 | 40.851 | 33.039 | 18.152 | 1.00 | 15.93 | N |
| ATOM | 3402 | CA | VAL | B | 210 | 39.464 | 33.445 | 18.378 | 1.00 | 16.36 | C |
| ATOM | 3403 | C | VAL | B | 210 | 39.339 | 34.974 | 18.345 | 1.00 | 16.58 | C |
| ATOM | 3404 | O | VAL | B | 210 | 38.386 | 35.517 | 17.781 | 1.00 | 16.56 | O |
| ATOM | 3405 | CB | VAL | B | 210 | 38.931 | 32.880 | 19.724 | 1.00 | 16.51 | C |
| ATOM | 3406 | CG1 | VAL | B | 210 | 37.569 | 33.472 | 20.088 | 1.00 | 16.71 | C |
| ATOM | 3407 | CG2 | VAL | B | 210 | 38.849 | 31.360 | 19.673 | 1.00 | 16.77 | C |
| ATOM | 3408 | N | TRP | B | 211 | 40.317 | 35.655 | 18.938 | 1.00 | 16.78 | N |
| ATOM | 3409 | CA | TRP | B | 211 | 40.376 | 37.113 | 18.938 | 1.00 | 17.07 | C |
| ATOM | 3410 | C | TRP | B | 211 | 40.483 | 37.664 | 17.514 | 1.00 | 17.46 | C |
| ATOM | 3411 | O | TRP | B | 211 | 39.771 | 38.603 | 17.158 | 1.00 | 17.73 | O |
| ATOM | 3412 | CB | TRP | B | 211 | 41.544 | 37.597 | 19.806 | 1.00 | 16.78 | C |
| ATOM | 3413 | CG | TRP | B | 211 | 41.634 | 39.088 | 19.961 | 1.00 | 16.05 | C |
| ATOM | 3414 | CD1 | TRP | B | 211 | 41.085 | 39.843 | 20.956 | 1.00 | 15.56 | C |
| ATOM | 3415 | NE1 | TRP | B | 211 | 41.391 | 41.170 | 20.769 | 1.00 | 15.38 | N |

FIG. 4EEE

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3416 | CE2 | TRP | B | 211 | 42.154 | 41.297 | 19.638 | 1.00 | 15.41 | C |
| ATOM | 3417 | CD2 | TRP | B | 211 | 42.329 | 40.002 | 19.103 | 1.00 | 15.73 | C |
| ATOM | 3418 | CE3 | TRP | B | 211 | 43.084 | 39.859 | 17.928 | 1.00 | 15.47 | C |
| ATOM | 3419 | CZ3 | TRP | B | 211 | 43.628 | 40.994 | 17.337 | 1.00 | 15.46 | C |
| ATOM | 3420 | CH2 | TRP | B | 211 | 43.435 | 42.268 | 17.898 | 1.00 | 15.36 | C |
| ATOM | 3421 | CZ2 | TRP | B | 211 | 42.701 | 42.440 | 19.043 | 1.00 | 15.19 | C |
| ATOM | 3422 | N | GLU | B | 212 | 41.365 | 37.070 | 16.711 | 1.00 | 17.88 | N |
| ATOM | 3423 | CA | GLU | B | 212 | 41.521 | 37.431 | 15.301 | 1.00 | 18.08 | C |
| ATOM | 3424 | C | GLU | B | 212 | 40.186 | 37.363 | 14.560 | 1.00 | 18.48 | C |
| ATOM | 3425 | O | GLU | B | 212 | 39.845 | 38.269 | 13.801 | 1.00 | 18.56 | O |
| ATOM | 3426 | CB | GLU | B | 212 | 42.512 | 36.488 | 14.617 | 1.00 | 18.02 | C |
| ATOM | 3427 | CG | GLU | B | 212 | 43.980 | 36.819 | 14.803 | 1.00 | 17.42 | C |
| ATOM | 3428 | CD | GLU | B | 212 | 44.875 | 35.756 | 14.194 | 1.00 | 17.22 | C |
| ATOM | 3429 | OE1 | GLU | B | 212 | 45.429 | 36.000 | 13.103 | 1.00 | 17.17 | O |
| ATOM | 3430 | OE2 | GLU | B | 212 | 45.016 | 34.670 | 14.796 | 1.00 | 17.09 | O |
| ATOM | 3431 | N | LEU | B | 213 | 39.441 | 36.284 | 14.792 | 1.00 | 19.08 | N |
| ATOM | 3432 | CA | LEU | B | 213 | 38.147 | 36.063 | 14.146 | 1.00 | 19.63 | C |
| ATOM | 3433 | C | LEU | B | 213 | 37.109 | 37.105 | 14.564 | 1.00 | 19.93 | C |
| ATOM | 3434 | O | LEU | B | 213 | 36.415 | 37.670 | 13.718 | 1.00 | 19.77 | O |
| ATOM | 3435 | CB | LEU | B | 213 | 37.629 | 34.646 | 14.438 | 1.00 | 19.47 | C |
| ATOM | 3436 | CG | LEU | B | 213 | 38.499 | 33.442 | 14.049 | 1.00 | 19.47 | C |
| ATOM | 3437 | CD1 | LEU | B | 213 | 37.819 | 32.133 | 14.436 | 1.00 | 19.58 | C |
| ATOM | 3438 | CD2 | LEU | B | 213 | 38.855 | 33.443 | 12.567 | 1.00 | 19.23 | C |
| ATOM | 3439 | N | MET | B | 214 | 37.027 | 37.359 | 15.869 | 1.00 | 20.48 | N |
| ATOM | 3440 | CA | MET | B | 214 | 36.051 | 38.290 | 16.438 | 1.00 | 20.92 | C |
| ATOM | 3441 | C | MET | B | 214 | 36.315 | 39.747 | 16.046 | 1.00 | 21.06 | C |
| ATOM | 3442 | O | MET | B | 214 | 35.396 | 40.566 | 16.015 | 1.00 | 21.08 | O |
| ATOM | 3443 | CB | MET | B | 214 | 36.008 | 38.151 | 17.963 | 1.00 | 21.01 | C |
| ATOM | 3444 | CG | MET | B | 214 | 35.669 | 36.750 | 18.460 | 1.00 | 21.37 | C |
| ATOM | 3445 | SD | MET | B | 214 | 33.983 | 36.252 | 18.092 | 1.00 | 22.53 | S |
| ATOM | 3446 | CE | MET | B | 214 | 34.060 | 34.474 | 18.422 | 1.00 | 22.44 | C |
| ATOM | 3447 | N | THR | B | 215 | 37.574 | 40.059 | 15.753 | 1.00 | 21.29 | N |
| ATOM | 3448 | CA | THR | B | 215 | 37.959 | 41.395 | 15.304 | 1.00 | 21.55 | C |
| ATOM | 3449 | C | THR | B | 215 | 38.001 | 41.468 | 13.775 | 1.00 | 21.77 | C |
| ATOM | 3450 | O | THR | B | 215 | 38.497 | 42.443 | 13.202 | 1.00 | 21.86 | O |
| ATOM | 3451 | CB | THR | B | 215 | 39.321 | 41.794 | 15.901 | 1.00 | 21.49 | C |
| ATOM | 3452 | OG1 | THR | B | 215 | 40.259 | 40.729 | 15.709 | 1.00 | 21.62 | O |
| ATOM | 3453 | CG2 | THR | B | 215 | 39.233 | 41.933 | 17.415 | 1.00 | 21.04 | C |
| ATOM | 3454 | N | PHE | B | 216 | 37.473 | 40.423 | 13.135 | 1.00 | 21.97 | N |
| ATOM | 3455 | CA | PHE | B | 216 | 37.373 | 40.306 | 11.674 | 1.00 | 22.06 | C |
| ATOM | 3456 | C | PHE | B | 216 | 38.714 | 40.402 | 10.930 | 1.00 | 22.12 | C |
| ATOM | 3457 | O | PHE | B | 216 | 38.783 | 40.927 | 9.815 | 1.00 | 21.87 | O |
| ATOM | 3458 | CB | PHE | B | 216 | 36.329 | 41.282 | 11.107 | 1.00 | 22.02 | C |
| ATOM | 3459 | CG | PHE | B | 216 | 34.921 | 40.995 | 11.559 | 1.00 | 21.79 | C |
| ATOM | 3460 | CD1 | PHE | B | 216 | 34.211 | 39.916 | 11.035 | 1.00 | 21.82 | C |
| ATOM | 3461 | CE1 | PHE | B | 216 | 32.908 | 39.649 | 11.449 | 1.00 | 21.43 | C |
| ATOM | 3462 | CZ | PHE | B | 216 | 32.305 | 40.467 | 12.399 | 1.00 | 21.50 | C |
| ATOM | 3463 | CE2 | PHE | B | 216 | 33.006 | 41.547 | 12.929 | 1.00 | 21.19 | C |
| ATOM | 3464 | CD2 | PHE | B | 216 | 34.304 | 41.805 | 12.508 | 1.00 | 21.41 | C |
| ATOM | 3465 | N | GLY | B | 217 | 39.770 | 39.895 | 11.563 | 1.00 | 22.38 | N |
| ATOM | 3466 | CA | GLY | B | 217 | 41.086 | 39.819 | 10.951 | 1.00 | 22.88 | C |
| ATOM | 3467 | C | GLY | B | 217 | 42.090 | 40.880 | 11.374 | 1.00 | 23.14 | C |
| ATOM | 3468 | O | GLY | B | 217 | 43.111 | 41.058 | 10.710 | 1.00 | 23.01 | O |
| ATOM | 3469 | N | SER | B | 218 | 41.808 | 41.578 | 12.473 | 1.00 | 23.62 | N |
| ATOM | 3470 | CA | SER | B | 218 | 42.713 | 42.598 | 13.008 | 1.00 | 24.15 | C |
| ATOM | 3471 | C | SER | B | 218 | 44.036 | 41.995 | 13.458 | 1.00 | 24.33 | C |
| ATOM | 3472 | O | SER | B | 218 | 44.075 | 40.876 | 13.974 | 1.00 | 24.36 | O |
| ATOM | 3473 | CB | SER | B | 218 | 42.071 | 43.342 | 14.182 | 1.00 | 24.10 | C |
| ATOM | 3474 | OG | SER | B | 218 | 40.835 | 43.924 | 13.808 | 1.00 | 24.72 | O |
| ATOM | 3475 | N | LYS | B | 219 | 45.112 | 42.748 | 13.254 | 1.00 | 24.82 | N |

FIG. 4FFF

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3476 | CA | LYS | B | 219 | 46.447 | 42.331 | 13.665 | 1.00 | 25.33 | C |
| ATOM | 3477 | C | LYS | B | 219 | 46.596 | 42.460 | 15.182 | 1.00 | 25.79 | C |
| ATOM | 3478 | O | LYS | B | 219 | 46.294 | 43.517 | 15.749 | 1.00 | 25.77 | O |
| ATOM | 3479 | CB | LYS | B | 219 | 47.517 | 43.159 | 12.949 | 1.00 | 25.30 | C |
| ATOM | 3480 | CG | LYS | B | 219 | 47.636 | 42.877 | 11.456 | 1.00 | 25.43 | C |
| ATOM | 3481 | CD | LYS | B | 219 | 47.908 | 44.151 | 10.665 | 1.00 | 25.36 | C |
| ATOM | 3482 | N | PRO | B | 220 | 47.033 | 41.381 | 15.838 | 1.00 | 26.26 | N |
| ATOM | 3483 | CA | PRO | B | 220 | 47.246 | 41.382 | 17.293 | 1.00 | 26.66 | C |
| ATOM | 3484 | C | PRO | B | 220 | 48.379 | 42.317 | 17.699 | 1.00 | 27.09 | C |
| ATOM | 3485 | O | PRO | B | 220 | 49.442 | 42.282 | 17.076 | 1.00 | 27.18 | O |
| ATOM | 3486 | CB | PRO | B | 220 | 47.626 | 39.927 | 17.593 | 1.00 | 26.49 | C |
| ATOM | 3487 | CG | PRO | B | 220 | 47.151 | 39.160 | 16.412 | 1.00 | 26.47 | C |
| ATOM | 3488 | CD | PRO | B | 220 | 47.342 | 40.070 | 15.240 | 1.00 | 26.18 | C |
| ATOM | 3489 | N | TYR | B | 221 | 48.145 | 43.136 | 18.725 | 1.00 | 27.68 | N |
| ATOM | 3490 | CA | TYR | B | 221 | 49.111 | 44.142 | 19.177 | 1.00 | 28.26 | C |
| ATOM | 3491 | C | TYR | B | 221 | 49.620 | 44.945 | 17.976 | 1.00 | 28.85 | C |
| ATOM | 3492 | O | TYR | B | 221 | 50.804 | 44.888 | 17.630 | 1.00 | 28.85 | O |
| ATOM | 3493 | CB | TYR | B | 221 | 50.277 | 43.498 | 19.945 | 1.00 | 28.09 | C |
| ATOM | 3494 | CG | TYR | B | 221 | 49.887 | 42.376 | 20.889 | 1.00 | 27.77 | C |
| ATOM | 3495 | CD1 | TYR | B | 221 | 49.532 | 42.642 | 22.211 | 1.00 | 27.47 | C |
| ATOM | 3496 | CE1 | TYR | B | 221 | 49.182 | 41.612 | 23.083 | 1.00 | 27.38 | C |
| ATOM | 3497 | CZ | TYR | B | 221 | 49.191 | 40.299 | 22.631 | 1.00 | 27.18 | C |
| ATOM | 3498 | OH | TYR | B | 221 | 48.844 | 39.276 | 23.484 | 1.00 | 26.85 | O |
| ATOM | 3499 | CE2 | TYR | B | 221 | 49.544 | 40.011 | 21.324 | 1.00 | 27.01 | C |
| ATOM | 3500 | CD2 | TYR | B | 221 | 49.894 | 41.045 | 20.464 | 1.00 | 27.41 | C |
| ATOM | 3501 | N | ASP | B | 222 | 48.701 | 45.686 | 17.357 | 1.00 | 29.68 | N |
| ATOM | 3502 | CA | ASP | B | 222 | 48.901 | 46.307 | 16.043 | 1.00 | 30.48 | C |
| ATOM | 3503 | C | ASP | B | 222 | 50.326 | 46.766 | 15.730 | 1.00 | 31.14 | C |
| ATOM | 3504 | O | ASP | B | 222 | 51.008 | 46.158 | 14.898 | 1.00 | 31.16 | O |
| ATOM | 3505 | CB | ASP | B | 222 | 47.911 | 47.455 | 15.829 | 1.00 | 30.52 | C |
| ATOM | 3506 | CG | ASP | B | 222 | 47.534 | 47.634 | 14.369 | 1.00 | 30.61 | C |
| ATOM | 3507 | OD1 | ASP | B | 222 | 48.443 | 47.744 | 13.519 | 1.00 | 30.55 | O |
| ATOM | 3508 | OD2 | ASP | B | 222 | 46.350 | 47.681 | 13.977 | 1.00 | 31.30 | O |
| ATOM | 3509 | N | GLY | B | 223 | 50.761 | 47.838 | 16.390 | 1.00 | 31.67 | N |
| ATOM | 3510 | CA | GLY | B | 223 | 52.038 | 48.460 | 16.086 | 1.00 | 32.55 | C |
| ATOM | 3511 | C | GLY | B | 223 | 53.112 | 48.272 | 17.140 | 1.00 | 33.14 | C |
| ATOM | 3512 | O | GLY | B | 223 | 54.102 | 49.006 | 17.155 | 1.00 | 33.45 | O |
| ATOM | 3513 | N | ILE | B | 224 | 52.917 | 47.293 | 18.020 | 1.00 | 33.50 | N |
| ATOM | 3514 | CA | ILE | B | 224 | 53.894 | 46.978 | 19.058 | 1.00 | 33.95 | C |
| ATOM | 3515 | C | ILE | B | 224 | 54.982 | 46.066 | 18.482 | 1.00 | 34.34 | C |
| ATOM | 3516 | O | ILE | B | 224 | 54.667 | 45.044 | 17.872 | 1.00 | 34.44 | O |
| ATOM | 3517 | CB | ILE | B | 224 | 53.202 | 46.301 | 20.277 | 1.00 | 33.94 | C |
| ATOM | 3518 | CG1 | ILE | B | 224 | 51.889 | 47.015 | 20.657 | 1.00 | 34.10 | C |
| ATOM | 3519 | CD1 | ILE | B | 224 | 52.038 | 48.421 | 21.246 | 1.00 | 34.20 | C |
| ATOM | 3520 | CG2 | ILE | B | 224 | 54.168 | 46.169 | 21.464 | 1.00 | 33.93 | C |
| ATOM | 3521 | N | PRO | B | 225 | 56.252 | 46.443 | 18.650 | 1.00 | 34.74 | N |
| ATOM | 3522 | CA | PRO | B | 225 | 57.378 | 45.577 | 18.269 | 1.00 | 34.92 | C |
| ATOM | 3523 | C | PRO | B | 225 | 57.420 | 44.292 | 19.093 | 1.00 | 35.07 | C |
| ATOM | 3524 | O | PRO | B | 225 | 57.064 | 44.309 | 20.272 | 1.00 | 35.07 | O |
| ATOM | 3525 | CB | PRO | B | 225 | 58.604 | 46.441 | 18.581 | 1.00 | 34.88 | C |
| ATOM | 3526 | CG | PRO | B | 225 | 58.088 | 47.837 | 18.589 | 1.00 | 34.90 | C |
| ATOM | 3527 | CD | PRO | B | 225 | 56.718 | 47.737 | 19.183 | 1.00 | 34.86 | C |
| ATOM | 3528 | N | ALA | B | 226 | 57.863 | 43.201 | 18.470 | 1.00 | 35.36 | N |
| ATOM | 3529 | CA | ALA | B | 226 | 57.872 | 41.876 | 19.098 | 1.00 | 35.42 | C |
| ATOM | 3530 | C | ALA | B | 226 | 58.869 | 41.741 | 20.257 | 1.00 | 35.54 | C |
| ATOM | 3531 | O | ALA | B | 226 | 58.947 | 40.690 | 20.898 | 1.00 | 35.78 | O |
| ATOM | 3532 | CB | ALA | B | 226 | 58.120 | 40.800 | 18.049 | 1.00 | 35.24 | C |
| ATOM | 3533 | N | SER | B | 227 | 59.619 | 42.807 | 20.520 | 1.00 | 35.60 | N |
| ATOM | 3534 | CA | SER | B | 227 | 60.585 | 42.836 | 21.617 | 1.00 | 35.62 | C |
| ATOM | 3535 | C | SER | B | 227 | 59.936 | 43.240 | 22.944 | 1.00 | 35.64 | C |

FIG. 4GGG

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3536 | O | SER | B | 227 | 60.443 | 42.908 | 24.019 | 1.00 | 35.51 | O |
| ATOM | 3537 | CB | SER | B | 227 | 61.739 | 43.786 | 21.287 | 1.00 | 35.69 | C |
| ATOM | 3538 | OG | SER | B | 227 | 61.760 | 44.119 | 19.908 | 1.00 | 35.66 | O |
| ATOM | 3539 | N | GLU | B | 228 | 58.806 | 43.939 | 22.854 | 1.00 | 35.65 | N |
| ATOM | 3540 | CA | GLU | B | 228 | 58.122 | 44.493 | 24.022 | 1.00 | 35.68 | C |
| ATOM | 3541 | C | GLU | B | 228 | 56.942 | 43.655 | 24.525 | 1.00 | 35.68 | C |
| ATOM | 3542 | O | GLU | B | 228 | 56.374 | 43.952 | 25.580 | 1.00 | 35.55 | O |
| ATOM | 3543 | CB | GLU | B | 228 | 57.651 | 45.919 | 23.718 | 1.00 | 35.71 | C |
| ATOM | 3544 | N | ILE | B | 229 | 56.590 | 42.608 | 23.779 | 1.00 | 35.78 | N |
| ATOM | 3545 | CA | ILE | B | 229 | 55.410 | 41.787 | 24.074 | 1.00 | 35.74 | C |
| ATOM | 3546 | C | ILE | B | 229 | 55.489 | 41.090 | 25.434 | 1.00 | 35.72 | C |
| ATOM | 3547 | O | ILE | B | 229 | 54.503 | 41.062 | 26.174 | 1.00 | 35.73 | O |
| ATOM | 3548 | CB | ILE | B | 229 | 55.145 | 40.754 | 22.932 | 1.00 | 35.77 | C |
| ATOM | 3549 | CG1 | ILE | B | 229 | 55.077 | 41.442 | 21.557 | 1.00 | 35.58 | C |
| ATOM | 3550 | CD1 | ILE | B | 229 | 53.839 | 42.312 | 21.316 | 1.00 | 35.50 | C |
| ATOM | 3551 | CG2 | ILE | B | 229 | 53.884 | 39.918 | 23.214 | 1.00 | 35.73 | C |
| ATOM | 3552 | N | SER | B | 230 | 56.660 | 40.545 | 25.760 | 1.00 | 35.78 | N |
| ATOM | 3553 | CA | SER | B | 230 | 56.864 | 39.820 | 27.018 | 1.00 | 35.82 | C |
| ATOM | 3554 | C | SER | B | 230 | 56.654 | 40.683 | 28.266 | 1.00 | 35.82 | C |
| ATOM | 3555 | O | SER | B | 230 | 56.065 | 40.225 | 29.245 | 1.00 | 35.86 | O |
| ATOM | 3556 | CB | SER | B | 230 | 58.244 | 39.154 | 27.050 | 1.00 | 35.84 | C |
| ATOM | 3557 | OG | SER | B | 230 | 59.286 | 40.115 | 27.044 | 1.00 | 36.16 | O |
| ATOM | 3558 | N | SER | B | 231 | 57.131 | 41.926 | 28.221 | 1.00 | 35.87 | N |
| ATOM | 3559 | CA | SER | B | 231 | 56.965 | 42.860 | 29.339 | 1.00 | 35.96 | C |
| ATOM | 3560 | C | SER | B | 231 | 55.520 | 43.353 | 29.461 | 1.00 | 35.89 | C |
| ATOM | 3561 | O | SER | B | 231 | 55.017 | 43.544 | 30.571 | 1.00 | 35.77 | O |
| ATOM | 3562 | CB | SER | B | 231 | 57.935 | 44.040 | 29.221 | 1.00 | 35.94 | C |
| ATOM | 3563 | OG | SER | B | 231 | 57.689 | 44.795 | 28.051 | 1.00 | 36.04 | O |
| ATOM | 3564 | N | ILE | B | 232 | 54.863 | 43.546 | 28.318 | 1.00 | 35.79 | N |
| ATOM | 3565 | CA | ILE | B | 232 | 53.441 | 43.887 | 28.283 | 1.00 | 35.86 | C |
| ATOM | 3566 | C | ILE | B | 232 | 52.573 | 42.777 | 28.885 | 1.00 | 35.90 | C |
| ATOM | 3567 | O | ILE | B | 232 | 51.584 | 43.058 | 29.567 | 1.00 | 36.04 | O |
| ATOM | 3568 | CB | ILE | B | 232 | 52.987 | 44.201 | 26.841 | 1.00 | 35.90 | C |
| ATOM | 3569 | N | LEU | B | 233 | 52.952 | 41.523 | 28.640 | 1.00 | 35.72 | N |
| ATOM | 3570 | CA | LEU | B | 233 | 52.237 | 40.381 | 29.206 | 1.00 | 35.69 | C |
| ATOM | 3571 | C | LEU | B | 233 | 52.535 | 40.203 | 30.692 | 1.00 | 35.77 | C |
| ATOM | 3572 | O | LEU | B | 233 | 51.651 | 39.830 | 31.467 | 1.00 | 35.85 | O |
| ATOM | 3573 | CB | LEU | B | 233 | 52.559 | 39.091 | 28.442 | 1.00 | 35.73 | C |
| ATOM | 3574 | CG | LEU | B | 233 | 52.033 | 38.944 | 27.008 | 1.00 | 35.60 | C |
| ATOM | 3575 | CD1 | LEU | B | 233 | 52.645 | 37.725 | 26.344 | 1.00 | 35.37 | C |
| ATOM | 3576 | CD2 | LEU | B | 233 | 50.510 | 38.882 | 26.963 | 1.00 | 35.43 | C |
| ATOM | 3577 | N | GLU | B | 234 | 53.781 | 40.474 | 31.080 | 1.00 | 35.90 | N |
| ATOM | 3578 | CA | GLU | B | 234 | 54.212 | 40.384 | 32.477 | 1.00 | 35.83 | C |
| ATOM | 3579 | C | GLU | B | 234 | 53.594 | 41.482 | 33.341 | 1.00 | 35.52 | C |
| ATOM | 3580 | O | GLU | B | 234 | 53.462 | 41.321 | 34.556 | 1.00 | 35.50 | O |
| ATOM | 3581 | CB | GLU | B | 234 | 55.739 | 40.430 | 32.577 | 1.00 | 36.07 | C |
| ATOM | 3582 | CG | GLU | B | 234 | 56.412 | 39.075 | 32.403 | 1.00 | 36.80 | C |
| ATOM | 3583 | CD | GLU | B | 234 | 57.862 | 39.177 | 31.958 | 1.00 | 37.64 | C |
| ATOM | 3584 | OE1 | GLU | B | 234 | 58.230 | 40.180 | 31.305 | 1.00 | 37.96 | O |
| ATOM | 3585 | OE2 | GLU | B | 234 | 58.639 | 38.243 | 32.259 | 1.00 | 37.97 | O |
| ATOM | 3586 | N | LYS | B | 235 | 53.221 | 42.593 | 32.706 | 1.00 | 35.08 | N |
| ATOM | 3587 | CA | LYS | B | 235 | 52.548 | 43.696 | 33.388 | 1.00 | 34.61 | C |
| ATOM | 3588 | C | LYS | B | 235 | 51.063 | 43.411 | 33.611 | 1.00 | 34.24 | C |
| ATOM | 3589 | O | LYS | B | 235 | 50.432 | 44.014 | 34.483 | 1.00 | 34.52 | O |
| ATOM | 3590 | CB | LYS | B | 235 | 52.726 | 45.001 | 32.607 | 1.00 | 34.66 | C |
| ATOM | 3591 | CG | LYS | B | 235 | 53.332 | 46.134 | 33.424 | 1.00 | 34.98 | C |
| ATOM | 3592 | CD | LYS | B | 235 | 54.856 | 46.200 | 33.279 | 1.00 | 34.96 | C |
| ATOM | 3593 | CE | LYS | B | 235 | 55.578 | 45.553 | 34.464 | 1.00 | 35.12 | C |
| ATOM | 3594 | NZ | LYS | B | 235 | 55.184 | 46.119 | 35.793 | 1.00 | 34.75 | N |
| ATOM | 3595 | N | GLY | B | 236 | 50.513 | 42.493 | 32.820 | 1.00 | 33.54 | N |

FIG. 4HHH

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3596 | CA | GLY | B | 236 | 49.120 | 42.105 | 32.943 | 1.00 | 32.71 | C |
| ATOM | 3597 | C | GLY | B | 236 | 48.246 | 42.638 | 31.826 | 1.00 | 32.27 | C |
| ATOM | 3598 | O | GLY | B | 236 | 47.019 | 42.584 | 31.917 | 1.00 | 32.22 | O |
| ATOM | 3599 | N | GLU | B | 237 | 48.877 | 43.154 | 30.772 | 1.00 | 31.81 | N |
| ATOM | 3600 | CA | GLU | B | 237 | 48.150 | 43.679 | 29.621 | 1.00 | 31.22 | C |
| ATOM | 3601 | C | GLU | B | 237 | 47.862 | 42.578 | 28.605 | 1.00 | 30.80 | C |
| ATOM | 3602 | O | GLU | B | 237 | 48.762 | 41.848 | 28.180 | 1.00 | 30.55 | O |
| ATOM | 3603 | CB | GLU | B | 237 | 48.914 | 44.833 | 28.965 | 1.00 | 31.35 | C |
| ATOM | 3604 | N | ARG | B | 238 | 46.593 | 42.469 | 28.230 | 1.00 | 30.23 | N |
| ATOM | 3605 | CA | ARG | B | 238 | 46.142 | 41.467 | 27.275 | 1.00 | 29.51 | C |
| ATOM | 3606 | C | ARG | B | 238 | 45.619 | 42.145 | 26.016 | 1.00 | 29.05 | C |
| ATOM | 3607 | O | ARG | B | 238 | 45.655 | 43.374 | 25.909 | 1.00 | 29.03 | O |
| ATOM | 3608 | CB | ARG | B | 238 | 45.059 | 40.587 | 27.911 | 1.00 | 29.53 | C |
| ATOM | 3609 | CG | ARG | B | 238 | 45.572 | 39.661 | 29.009 | 1.00 | 29.53 | C |
| ATOM | 3610 | CD | ARG | B | 238 | 46.682 | 38.722 | 28.553 | 1.00 | 29.54 | C |
| ATOM | 3611 | NE | ARG | B | 238 | 47.386 | 38.081 | 29.662 | 1.00 | 29.35 | N |
| ATOM | 3612 | CZ | ARG | B | 238 | 48.448 | 38.588 | 30.280 | 1.00 | 29.15 | C |
| ATOM | 3613 | NH1 | ARG | B | 238 | 49.016 | 37.917 | 31.271 | 1.00 | 29.29 | N |
| ATOM | 3614 | NH2 | ARG | B | 238 | 48.942 | 39.764 | 29.921 | 1.00 | 28.79 | N |
| ATOM | 3615 | N | LEU | B | 239 | 45.153 | 41.341 | 25.061 | 1.00 | 28.36 | N |
| ATOM | 3616 | CA | LEU | B | 239 | 44.513 | 41.859 | 23.855 | 1.00 | 27.69 | C |
| ATOM | 3617 | C | LEU | B | 239 | 43.159 | 42.462 | 24.219 | 1.00 | 27.28 | C |
| ATOM | 3618 | O | LEU | B | 239 | 42.451 | 41.915 | 25.065 | 1.00 | 27.37 | O |
| ATOM | 3619 | CB | LEU | B | 239 | 44.342 | 40.750 | 22.814 | 1.00 | 27.61 | C |
| ATOM | 3620 | CG | LEU | B | 239 | 45.575 | 40.346 | 22.001 | 1.00 | 27.34 | C |
| ATOM | 3621 | CD1 | LEU | B | 239 | 45.458 | 38.901 | 21.535 | 1.00 | 27.11 | C |
| ATOM | 3622 | CD2 | LEU | B | 239 | 45.788 | 41.277 | 20.817 | 1.00 | 26.93 | C |
| ATOM | 3623 | N | PRO | B | 240 | 42.801 | 43.586 | 23.593 | 1.00 | 26.91 | N |
| ATOM | 3624 | CA | PRO | B | 240 | 41.571 | 44.308 | 23.945 | 1.00 | 26.60 | C |
| ATOM | 3625 | C | PRO | B | 240 | 40.304 | 43.538 | 23.588 | 1.00 | 26.38 | C |
| ATOM | 3626 | O | PRO | B | 240 | 40.332 | 42.697 | 22.688 | 1.00 | 26.35 | O |
| ATOM | 3627 | CB | PRO | B | 240 | 41.667 | 45.588 | 23.107 | 1.00 | 26.56 | C |
| ATOM | 3628 | CG | PRO | B | 240 | 42.535 | 45.230 | 21.961 | 1.00 | 26.48 | C |
| ATOM | 3629 | CD | PRO | B | 240 | 43.533 | 44.253 | 22.500 | 1.00 | 26.91 | C |
| ATOM | 3630 | N | GLN | B | 241 | 39.215 | 43.825 | 24.298 | 1.00 | 26.12 | N |
| ATOM | 3631 | CA | GLN | B | 241 | 37.916 | 43.221 | 24.018 | 1.00 | 25.84 | C |
| ATOM | 3632 | C | GLN | B | 241 | 37.402 | 43.664 | 22.649 | 1.00 | 25.72 | C |
| ATOM | 3633 | O | GLN | B | 241 | 37.301 | 44.864 | 22.384 | 1.00 | 25.98 | O |
| ATOM | 3634 | CB | GLN | B | 241 | 36.905 | 43.582 | 25.111 | 1.00 | 25.79 | C |
| ATOM | 3635 | CG | GLN | B | 241 | 35.552 | 42.887 | 24.977 | 1.00 | 25.44 | C |
| ATOM | 3636 | CD | GLN | B | 241 | 34.592 | 43.211 | 26.113 | 1.00 | 25.15 | C |
| ATOM | 3637 | OE1 | GLN | B | 241 | 34.977 | 43.814 | 27.114 | 1.00 | 24.87 | O |
| ATOM | 3638 | NE2 | GLN | B | 241 | 33.338 | 42.804 | 25.957 | 1.00 | 25.48 | N |
| ATOM | 3639 | N | PRO | B | 242 | 37.102 | 42.697 | 21.781 | 1.00 | 25.53 | N |
| ATOM | 3640 | CA | PRO | B | 242 | 36.520 | 42.985 | 20.463 | 1.00 | 25.41 | C |
| ATOM | 3641 | C | PRO | B | 242 | 35.138 | 43.639 | 20.569 | 1.00 | 25.21 | C |
| ATOM | 3642 | O | PRO | B | 242 | 34.315 | 43.179 | 21.362 | 1.00 | 24.97 | O |
| ATOM | 3643 | CB | PRO | B | 242 | 36.406 | 41.597 | 19.822 | 1.00 | 25.42 | C |
| ATOM | 3644 | CG | PRO | B | 242 | 37.384 | 40.756 | 20.570 | 1.00 | 25.45 | C |
| ATOM | 3645 | CD | PRO | B | 242 | 37.318 | 41.253 | 21.980 | 1.00 | 25.44 | C |
| ATOM | 3646 | N | PRO | B | 243 | 34.900 | 44.697 | 19.790 | 1.00 | 25.22 | N |
| ATOM | 3647 | CA | PRO | B | 243 | 33.629 | 45.435 | 19.820 | 1.00 | 25.23 | C |
| ATOM | 3648 | C | PRO | B | 243 | 32.366 | 44.575 | 19.719 | 1.00 | 25.20 | C |
| ATOM | 3649 | O | PRO | B | 243 | 31.361 | 44.968 | 20.304 | 1.00 | 25.32 | O |
| ATOM | 3650 | CB | PRO | B | 243 | 33.738 | 46.361 | 18.607 | 1.00 | 25.15 | C |
| ATOM | 3651 | CG | PRO | B | 243 | 35.186 | 46.595 | 18.462 | 1.00 | 25.16 | C |
| ATOM | 3652 | CD | PRO | B | 243 | 35.849 | 45.294 | 18.831 | 1.00 | 25.26 | C |
| ATOM | 3653 | N | ILE | B | 244 | 32.412 | 43.446 | 19.014 | 1.00 | 25.18 | N |
| ATOM | 3654 | CA | ILE | B | 244 | 31.235 | 42.577 | 18.874 | 1.00 | 25.21 | C |
| ATOM | 3655 | C | ILE | B | 244 | 31.034 | 41.618 | 20.055 | 1.00 | 25.29 | C |

FIG. 4III

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3656 | O | ILE | B | 244 | 29.957 | 41.032 | 20.209 | 1.00 | 25.56 | O |
| ATOM | 3657 | CB | ILE | B | 244 | 31.267 | 41.774 | 17.537 | 1.00 | 25.23 | C |
| ATOM | 3658 | CG1 | ILE | B | 244 | 32.432 | 40.775 | 17.517 | 1.00 | 25.07 | C |
| ATOM | 3659 | CD1 | ILE | B | 244 | 32.108 | 39.464 | 16.823 | 1.00 | 24.83 | C |
| ATOM | 3660 | CG2 | ILE | B | 244 | 31.292 | 42.713 | 16.325 | 1.00 | 25.08 | C |
| ATOM | 3661 | N | CYS | B | 245 | 32.065 | 41.475 | 20.885 | 1.00 | 25.13 | N |
| ATOM | 3662 | CA | CYS | B | 245 | 32.097 | 40.455 | 21.932 | 1.00 | 24.91 | C |
| ATOM | 3663 | C | CYS | B | 245 | 31.433 | 40.870 | 23.235 | 1.00 | 24.82 | C |
| ATOM | 3664 | O | CYS | B | 245 | 31.682 | 41.963 | 23.745 | 1.00 | 25.06 | O |
| ATOM | 3665 | CB | CYS | B | 245 | 33.544 | 40.059 | 22.232 | 1.00 | 24.87 | C |
| ATOM | 3666 | SG | CYS | B | 245 | 34.222 | 38.824 | 21.117 | 1.00 | 24.95 | S |
| ATOM | 3667 | N | THR | B | 246 | 30.605 | 39.979 | 23.777 | 1.00 | 24.67 | N |
| ATOM | 3668 | CA | THR | B | 246 | 30.121 | 40.106 | 25.154 | 1.00 | 24.56 | C |
| ATOM | 3669 | C | THR | B | 246 | 31.246 | 39.717 | 26.103 | 1.00 | 24.45 | C |
| ATOM | 3670 | O | THR | B | 246 | 32.233 | 39.108 | 25.681 | 1.00 | 24.60 | O |
| ATOM | 3671 | CB | THR | B | 246 | 28.908 | 39.190 | 25.410 | 1.00 | 24.47 | C |
| ATOM | 3672 | OG1 | THR | B | 246 | 29.211 | 37.860 | 24.973 | 1.00 | 24.53 | O |
| ATOM | 3673 | CG2 | THR | B | 246 | 27.716 | 39.600 | 24.553 | 1.00 | 24.30 | C |
| ATOM | 3674 | N | ILE | B | 247 | 31.095 | 40.057 | 27.383 | 1.00 | 24.22 | N |
| ATOM | 3675 | CA | ILE | B | 247 | 32.096 | 39.704 | 28.392 | 1.00 | 24.03 | C |
| ATOM | 3676 | C | ILE | B | 247 | 32.222 | 38.182 | 28.580 | 1.00 | 23.94 | C |
| ATOM | 3677 | O | ILE | B | 247 | 33.278 | 37.689 | 28.974 | 1.00 | 23.84 | O |
| ATOM | 3678 | CB | ILE | B | 247 | 31.844 | 40.461 | 29.734 | 1.00 | 23.96 | C |
| ATOM | 3679 | CG1 | ILE | B | 247 | 33.084 | 40.407 | 30.633 | 1.00 | 24.08 | C |
| ATOM | 3680 | CD1 | ILE | B | 247 | 33.890 | 41.685 | 30.652 | 1.00 | 24.75 | C |
| ATOM | 3681 | CG2 | ILE | B | 247 | 30.603 | 39.932 | 30.463 | 1.00 | 24.05 | C |
| ATOM | 3682 | N | ASP | B | 248 | 31.147 | 37.455 | 28.268 | 1.00 | 23.94 | N |
| ATOM | 3683 | CA | ASP | B | 248 | 31.139 | 35.991 | 28.286 | 1.00 | 23.92 | C |
| ATOM | 3684 | C | ASP | B | 248 | 32.221 | 35.417 | 27.369 | 1.00 | 24.01 | C |
| ATOM | 3685 | O | ASP | B | 248 | 33.051 | 34.619 | 27.806 | 1.00 | 24.07 | O |
| ATOM | 3686 | CB | ASP | B | 248 | 29.769 | 35.447 | 27.861 | 1.00 | 23.91 | C |
| ATOM | 3687 | CG | ASP | B | 248 | 28.609 | 36.160 | 28.537 | 1.00 | 24.03 | C |
| ATOM | 3688 | OD1 | ASP | B | 248 | 28.381 | 37.355 | 28.245 | 1.00 | 23.78 | O |
| ATOM | 3689 | OD2 | ASP | B | 248 | 27.861 | 35.598 | 29.365 | 1.00 | 24.27 | O |
| ATOM | 3690 | N | VAL | B | 249 | 32.206 | 35.836 | 26.104 | 1.00 | 24.12 | N |
| ATOM | 3691 | CA | VAL | B | 249 | 33.174 | 35.369 | 25.108 | 1.00 | 24.25 | C |
| ATOM | 3692 | C | VAL | B | 249 | 34.576 | 35.929 | 25.378 | 1.00 | 24.44 | C |
| ATOM | 3693 | O | VAL | B | 249 | 35.574 | 35.223 | 25.199 | 1.00 | 24.79 | O |
| ATOM | 3694 | CB | VAL | B | 249 | 32.723 | 35.695 | 23.650 | 1.00 | 24.18 | C |
| ATOM | 3695 | CG1 | VAL | B | 249 | 33.731 | 35.177 | 22.635 | 1.00 | 23.89 | C |
| ATOM | 3696 | CG2 | VAL | B | 249 | 31.350 | 35.099 | 23.358 | 1.00 | 23.95 | C |
| ATOM | 3697 | N | TYR | B | 250 | 34.647 | 37.186 | 25.816 | 1.00 | 24.26 | N |
| ATOM | 3698 | CA | TYR | B | 250 | 35.929 | 37.817 | 26.126 | 1.00 | 24.14 | C |
| ATOM | 3699 | C | TYR | B | 250 | 36.645 | 37.172 | 27.319 | 1.00 | 24.25 | C |
| ATOM | 3700 | O | TYR | B | 250 | 37.872 | 37.081 | 27.330 | 1.00 | 24.26 | O |
| ATOM | 3701 | CB | TYR | B | 250 | 35.770 | 39.326 | 26.345 | 1.00 | 23.90 | C |
| ATOM | 3702 | CG | TYR | B | 250 | 37.084 | 40.050 | 26.576 | 1.00 | 23.47 | C |
| ATOM | 3703 | CD1 | TYR | B | 250 | 37.255 | 40.887 | 27.678 | 1.00 | 23.11 | C |
| ATOM | 3704 | CE1 | TYR | B | 250 | 38.462 | 41.549 | 27.899 | 1.00 | 22.88 | C |
| ATOM | 3705 | CZ | TYR | B | 250 | 39.511 | 41.375 | 27.009 | 1.00 | 22.92 | C |
| ATOM | 3706 | OH | TYR | B | 250 | 40.705 | 42.026 | 27.222 | 1.00 | 22.75 | O |
| ATOM | 3707 | CE2 | TYR | B | 250 | 39.368 | 40.544 | 25.909 | 1.00 | 22.93 | C |
| ATOM | 3708 | CD2 | TYR | B | 250 | 38.159 | 39.890 | 25.696 | 1.00 | 23.00 | C |
| ATOM | 3709 | N | MET | B | 251 | 35.880 | 36.719 | 28.310 | 1.00 | 24.41 | N |
| ATOM | 3710 | CA | MET | B | 251 | 36.456 | 36.053 | 29.479 | 1.00 | 24.57 | C |
| ATOM | 3711 | C | MET | B | 251 | 37.110 | 34.713 | 29.148 | 1.00 | 24.63 | C |
| ATOM | 3712 | O | MET | B | 251 | 38.071 | 34.312 | 29.807 | 1.00 | 24.55 | O |
| ATOM | 3713 | CB | MET | B | 251 | 35.417 | 35.875 | 30.585 | 1.00 | 24.68 | C |
| ATOM | 3714 | CG | MET | B | 251 | 35.901 | 36.350 | 31.942 | 1.00 | 24.76 | C |
| ATOM | 3715 | SD | MET | B | 251 | 36.242 | 38.117 | 31.953 | 1.00 | 25.31 | S |

FIG. 4JJJ

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3716 | CE | MET | B | 251 | 37.961 | 38.126 | 32.390 | 1.00 | 24.63 | C |
| ATOM | 3717 | N | ILE | B | 252 | 36.582 | 34.027 | 28.135 | 1.00 | 24.73 | N |
| ATOM | 3718 | CA | ILE | B | 252 | 37.204 | 32.813 | 27.608 | 1.00 | 24.72 | C |
| ATOM | 3719 | C | ILE | B | 252 | 38.610 | 33.137 | 27.103 | 1.00 | 24.59 | C |
| ATOM | 3720 | O | ILE | B | 252 | 39.572 | 32.452 | 27.449 | 1.00 | 24.57 | O |
| ATOM | 3721 | CB | ILE | B | 252 | 36.335 | 32.191 | 26.483 | 1.00 | 24.77 | C |
| ATOM | 3722 | CG1 | ILE | B | 252 | 35.067 | 31.564 | 27.069 | 1.00 | 24.97 | C |
| ATOM | 3723 | CD1 | ILE | B | 252 | 33.921 | 31.454 | 26.081 | 1.00 | 25.20 | C |
| ATOM | 3724 | CG2 | ILE | B | 252 | 37.120 | 31.146 | 25.694 | 1.00 | 24.63 | C |
| ATOM | 3725 | N | MET | B | 253 | 38.711 | 34.201 | 26.307 | 1.00 | 24.61 | N |
| ATOM | 3726 | CA | MET | B | 253 | 39.978 | 34.652 | 25.735 | 1.00 | 24.61 | C |
| ATOM | 3727 | C | MET | B | 253 | 41.000 | 35.017 | 26.814 | 1.00 | 24.57 | C |
| ATOM | 3728 | O | MET | B | 253 | 42.156 | 34.591 | 26.746 | 1.00 | 24.60 | O |
| ATOM | 3729 | CB | MET | B | 253 | 39.749 | 35.845 | 24.800 | 1.00 | 24.68 | C |
| ATOM | 3730 | CG | MET | B | 253 | 39.200 | 35.486 | 23.429 | 1.00 | 24.47 | C |
| ATOM | 3731 | SD | MET | B | 253 | 38.876 | 36.958 | 22.437 | 1.00 | 24.97 | S |
| ATOM | 3732 | CE | MET | B | 253 | 37.146 | 36.767 | 22.081 | 1.00 | 24.50 | C |
| ATOM | 3733 | N | VAL | B | 254 | 40.562 | 35.796 | 27.803 | 1.00 | 24.43 | N |
| ATOM | 3734 | CA | VAL | B | 254 | 41.411 | 36.196 | 28.928 | 1.00 | 24.22 | C |
| ATOM | 3735 | C | VAL | B | 254 | 41.940 | 34.970 | 29.672 | 1.00 | 24.26 | C |
| ATOM | 3736 | O | VAL | B | 254 | 43.120 | 34.915 | 30.026 | 1.00 | 24.29 | O |
| ATOM | 3737 | CB | VAL | B | 254 | 40.661 | 37.149 | 29.903 | 1.00 | 24.23 | C |
| ATOM | 3738 | CG1 | VAL | B | 254 | 41.502 | 37.460 | 31.141 | 1.00 | 23.78 | C |
| ATOM | 3739 | CG2 | VAL | B | 254 | 40.265 | 38.445 | 29.196 | 1.00 | 24.23 | C |
| ATOM | 3740 | N | LYS | B | 255 | 41.064 | 33.987 | 29.884 | 1.00 | 24.32 | N |
| ATOM | 3741 | CA | LYS | B | 255 | 41.418 | 32.739 | 30.561 | 1.00 | 24.48 | C |
| ATOM | 3742 | C | LYS | B | 255 | 42.479 | 31.950 | 29.799 | 1.00 | 24.46 | C |
| ATOM | 3743 | O | LYS | B | 255 | 43.288 | 31.253 | 30.405 | 1.00 | 24.53 | O |
| ATOM | 3744 | CB | LYS | B | 255 | 40.180 | 31.866 | 30.766 | 1.00 | 24.59 | C |
| ATOM | 3745 | CG | LYS | B | 255 | 39.359 | 32.211 | 31.998 | 1.00 | 25.26 | C |
| ATOM | 3746 | CD | LYS | B | 255 | 38.444 | 31.059 | 32.392 | 1.00 | 25.97 | C |
| ATOM | 3747 | CE | LYS | B | 255 | 37.128 | 31.102 | 31.622 | 1.00 | 26.83 | C |
| ATOM | 3748 | NZ | LYS | B | 255 | 36.307 | 29.878 | 31.845 | 1.00 | 27.09 | N |
| ATOM | 3749 | N | CYS | B | 256 | 42.469 | 32.062 | 28.471 | 1.00 | 24.37 | N |
| ATOM | 3750 | CA | CYS | B | 256 | 43.485 | 31.423 | 27.638 | 1.00 | 24.31 | C |
| ATOM | 3751 | C | CYS | B | 256 | 44.857 | 32.097 | 27.778 | 1.00 | 24.28 | C |
| ATOM | 3752 | O | CYS | B | 256 | 45.881 | 31.490 | 27.466 | 1.00 | 24.08 | O |
| ATOM | 3753 | CB | CYS | B | 256 | 43.049 | 31.400 | 26.170 | 1.00 | 24.16 | C |
| ATOM | 3754 | SG | CYS | B | 256 | 41.586 | 30.394 | 25.828 | 1.00 | 24.07 | S |
| ATOM | 3755 | N | TRP | B | 257 | 44.868 | 33.343 | 28.253 | 1.00 | 24.42 | N |
| ATOM | 3756 | CA | TRP | B | 257 | 46.106 | 34.122 | 28.360 | 1.00 | 24.78 | C |
| ATOM | 3757 | C | TRP | B | 257 | 46.595 | 34.340 | 29.804 | 1.00 | 24.89 | C |
| ATOM | 3758 | O | TRP | B | 257 | 47.131 | 35.399 | 30.135 | 1.00 | 24.88 | O |
| ATOM | 3759 | CB | TRP | B | 257 | 45.969 | 35.471 | 27.638 | 1.00 | 24.62 | C |
| ATOM | 3760 | CG | TRP | B | 257 | 45.406 | 35.408 | 26.242 | 1.00 | 24.90 | C |
| ATOM | 3761 | CD1 | TRP | B | 257 | 45.695 | 34.486 | 25.273 | 1.00 | 24.93 | C |
| ATOM | 3762 | NE1 | TRP | B | 257 | 44.989 | 34.764 | 24.127 | 1.00 | 25.14 | N |
| ATOM | 3763 | CE2 | TRP | B | 257 | 44.226 | 35.883 | 24.332 | 1.00 | 25.19 | C |
| ATOM | 3764 | CD2 | TRP | B | 257 | 44.469 | 36.320 | 25.655 | 1.00 | 25.19 | C |
| ATOM | 3765 | CE3 | TRP | B | 257 | 43.797 | 37.464 | 26.116 | 1.00 | 24.95 | C |
| ATOM | 3766 | CZ3 | TRP | B | 257 | 42.924 | 38.123 | 25.257 | 1.00 | 25.02 | C |
| ATOM | 3767 | CH2 | TRP | B | 257 | 42.711 | 37.664 | 23.946 | 1.00 | 24.95 | C |
| ATOM | 3768 | CZ2 | TRP | B | 257 | 43.348 | 36.549 | 23.468 | 1.00 | 25.07 | C |
| ATOM | 3769 | N | MET | B | 258 | 46.421 | 33.331 | 30.653 | 1.00 | 25.25 | N |
| ATOM | 3770 | CA | MET | B | 258 | 46.883 | 33.404 | 32.039 | 1.00 | 25.54 | C |
| ATOM | 3771 | C | MET | B | 258 | 48.317 | 32.896 | 32.159 | 1.00 | 25.63 | C |
| ATOM | 3772 | O | MET | B | 258 | 48.696 | 31.938 | 31.482 | 1.00 | 25.71 | O |
| ATOM | 3773 | CB | MET | B | 258 | 45.956 | 32.611 | 32.965 | 1.00 | 25.60 | C |
| ATOM | 3774 | CG | MET | B | 258 | 44.499 | 33.032 | 32.887 | 1.00 | 25.97 | C |
| ATOM | 3775 | SD | MET | B | 258 | 43.726 | 33.239 | 34.491 | 1.00 | 26.80 | S |

FIG. 4KKK

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3776 | CE | MET | B | 258 | 42.833 | 34.773 | 34.239 | 1.00 | 26.84 | C |
| ATOM | 3777 | N | ILE | B | 259 | 49.105 | 33.544 | 33.018 | 1.00 | 25.78 | N |
| ATOM | 3778 | CA | ILE | B | 259 | 50.520 | 33.200 | 33.200 | 1.00 | 25.96 | C |
| ATOM | 3779 | C | ILE | B | 259 | 50.678 | 31.740 | 33.618 | 1.00 | 25.96 | C |
| ATOM | 3780 | O | ILE | B | 259 | 51.483 | 31.006 | 33.044 | 1.00 | 26.06 | O |
| ATOM | 3781 | CB | ILE | B | 259 | 51.212 | 34.151 | 34.220 | 1.00 | 25.92 | C |
| ATOM | 3782 | CG1 | ILE | B | 259 | 50.980 | 35.628 | 33.858 | 1.00 | 26.17 | C |
| ATOM | 3783 | CD1 | ILE | B | 259 | 51.630 | 36.095 | 32.551 | 1.00 | 26.28 | C |
| ATOM | 3784 | CG2 | ILE | B | 259 | 52.706 | 33.841 | 34.333 | 1.00 | 26.02 | C |
| ATOM | 3785 | N | ASP | B | 260 | 49.898 | 31.336 | 34.615 | 1.00 | 26.12 | N |
| ATOM | 3786 | CA | ASP | B | 260 | 49.836 | 29.950 | 35.052 | 1.00 | 26.15 | C |
| ATOM | 3787 | C | ASP | B | 260 | 49.059 | 29.138 | 34.019 | 1.00 | 26.37 | C |
| ATOM | 3788 | O | ASP | B | 260 | 47.860 | 29.359 | 33.811 | 1.00 | 26.43 | O |
| ATOM | 3789 | CB | ASP | B | 260 | 49.182 | 29.863 | 36.436 | 1.00 | 26.04 | C |
| ATOM | 3790 | CG | ASP | B | 260 | 48.973 | 28.433 | 36.906 | 1.00 | 26.23 | C |
| ATOM | 3791 | OD1 | ASP | B | 260 | 47.947 | 28.177 | 37.572 | 1.00 | 26.35 | O |
| ATOM | 3792 | OD2 | ASP | B | 260 | 49.773 | 27.501 | 36.669 | 1.00 | 26.31 | O |
| ATOM | 3793 | N | ALA | B | 261 | 49.758 | 28.206 | 33.372 | 1.00 | 26.54 | N |
| ATOM | 3794 | CA | ALA | B | 261 | 49.189 | 27.369 | 32.315 | 1.00 | 26.58 | C |
| ATOM | 3795 | C | ALA | B | 261 | 48.043 | 26.484 | 32.805 | 1.00 | 26.73 | C |
| ATOM | 3796 | O | ALA | B | 261 | 47.130 | 26.160 | 32.040 | 1.00 | 26.72 | O |
| ATOM | 3797 | CB | ALA | B | 261 | 50.275 | 26.522 | 31.674 | 1.00 | 26.47 | C |
| ATOM | 3798 | N | ASP | B | 262 | 48.100 | 26.104 | 34.081 | 1.00 | 26.87 | N |
| ATOM | 3799 | CA | ASP | B | 262 | 47.091 | 25.245 | 34.701 | 1.00 | 26.98 | C |
| ATOM | 3800 | C | ASP | B | 262 | 45.716 | 25.912 | 34.766 | 1.00 | 26.83 | C |
| ATOM | 3801 | O | ASP | B | 262 | 44.686 | 25.241 | 34.653 | 1.00 | 27.04 | O |
| ATOM | 3802 | CB | ASP | B | 262 | 47.537 | 24.834 | 36.105 | 1.00 | 27.19 | C |
| ATOM | 3803 | CG | ASP | B | 262 | 48.790 | 23.974 | 36.093 | 1.00 | 27.88 | C |
| ATOM | 3804 | OD1 | ASP | B | 262 | 49.868 | 24.480 | 36.481 | 1.00 | 27.90 | O |
| ATOM | 3805 | OD2 | ASP | B | 262 | 48.790 | 22.781 | 35.714 | 1.00 | 28.45 | O |
| ATOM | 3806 | N | SER | B | 263 | 45.712 | 27.231 | 34.941 | 1.00 | 26.47 | N |
| ATOM | 3807 | CA | SER | B | 263 | 44.480 | 28.003 | 35.063 | 1.00 | 26.00 | C |
| ATOM | 3808 | C | SER | B | 263 | 43.765 | 28.202 | 33.723 | 1.00 | 25.73 | C |
| ATOM | 3809 | O | SER | B | 263 | 42.572 | 28.516 | 33.695 | 1.00 | 25.93 | O |
| ATOM | 3810 | CB | SER | B | 263 | 44.768 | 29.352 | 35.722 | 1.00 | 26.12 | C |
| ATOM | 3811 | OG | SER | B | 263 | 45.106 | 29.182 | 37.090 | 1.00 | 26.04 | O |
| ATOM | 3812 | N | ARG | B | 264 | 44.497 | 28.019 | 32.624 | 1.00 | 25.11 | N |
| ATOM | 3813 | CA | ARG | B | 264 | 43.930 | 28.092 | 31.275 | 1.00 | 24.40 | C |
| ATOM | 3814 | C | ARG | B | 264 | 42.929 | 26.958 | 31.031 | 1.00 | 24.16 | C |
| ATOM | 3815 | O | ARG | B | 264 | 43.097 | 25.862 | 31.570 | 1.00 | 24.04 | O |
| ATOM | 3816 | CB | ARG | B | 264 | 45.037 | 28.024 | 30.222 | 1.00 | 24.15 | C |
| ATOM | 3817 | CG | ARG | B | 264 | 45.965 | 29.215 | 30.195 | 1.00 | 23.52 | C |
| ATOM | 3818 | CD | ARG | B | 264 | 47.111 | 29.068 | 29.216 | 1.00 | 22.50 | C |
| ATOM | 3819 | NE | ARG | B | 264 | 48.246 | 29.902 | 29.591 | 1.00 | 21.91 | N |
| ATOM | 3820 | CZ | ARG | B | 264 | 49.502 | 29.661 | 29.248 | 1.00 | 21.59 | C |
| ATOM | 3821 | NH1 | ARG | B | 264 | 50.463 | 30.483 | 29.645 | 1.00 | 21.71 | N |
| ATOM | 3822 | NH2 | ARG | B | 264 | 49.804 | 28.603 | 28.508 | 1.00 | 21.46 | N |
| ATOM | 3823 | N | PRO | B | 265 | 41.895 | 27.218 | 30.227 | 1.00 | 23.89 | N |
| ATOM | 3824 | CA | PRO | B | 265 | 40.892 | 26.198 | 29.897 | 1.00 | 23.77 | C |
| ATOM | 3825 | C | PRO | B | 265 | 41.477 | 25.020 | 29.123 | 1.00 | 23.71 | C |
| ATOM | 3826 | O | PRO | B | 265 | 42.526 | 25.146 | 28.486 | 1.00 | 23.83 | O |
| ATOM | 3827 | CB | PRO | B | 265 | 39.900 | 26.954 | 29.003 | 1.00 | 23.74 | C |
| ATOM | 3828 | CG | PRO | B | 265 | 40.136 | 28.388 | 29.279 | 1.00 | 23.61 | C |
| ATOM | 3829 | CD | PRO | B | 265 | 41.591 | 28.507 | 29.579 | 1.00 | 23.87 | C |
| ATOM | 3830 | N | LYS | B | 266 | 40.797 | 23.883 | 29.192 | 1.00 | 23.61 | N |
| ATOM | 3831 | CA | LYS | B | 266 | 41.151 | 22.722 | 28.388 | 1.00 | 23.45 | C |
| ATOM | 3832 | C | LYS | B | 266 | 40.340 | 22.762 | 27.096 | 1.00 | 23.38 | C |
| ATOM | 3833 | O | LYS | B | 266 | 39.217 | 23.277 | 27.082 | 1.00 | 23.33 | O |
| ATOM | 3834 | CB | LYS | B | 266 | 40.870 | 21.429 | 29.161 | 1.00 | 23.47 | C |
| ATOM | 3835 | CG | LYS | B | 266 | 41.887 | 21.114 | 30.249 | 1.00 | 23.14 | C |

FIG. 4LLL

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3836 | N | PHE | B | 267 | 40.905 | 22.220 | 26.018 | 1.00 | 23.21 | N |
| ATOM | 3837 | CA | PHE | B | 267 | 40.234 | 22.219 | 24.714 | 1.00 | 23.23 | C |
| ATOM | 3838 | C | PHE | B | 267 | 38.878 | 21.510 | 24.739 | 1.00 | 23.35 | C |
| ATOM | 3839 | O | PHE | B | 267 | 37.957 | 21.897 | 24.013 | 1.00 | 23.52 | O |
| ATOM | 3840 | CB | PHE | B | 267 | 41.134 | 21.622 | 23.626 | 1.00 | 23.04 | C |
| ATOM | 3841 | CG | PHE | B | 267 | 42.172 | 22.580 | 23.102 | 1.00 | 22.55 | C |
| ATOM | 3842 | CD1 | PHE | B | 267 | 41.797 | 23.779 | 22.502 | 1.00 | 21.94 | C |
| ATOM | 3843 | CE1 | PHE | B | 267 | 42.755 | 24.669 | 22.022 | 1.00 | 21.64 | C |
| ATOM | 3844 | CZ | PHE | B | 267 | 44.105 | 24.360 | 22.136 | 1.00 | 21.59 | C |
| ATOM | 3845 | CE2 | PHE | B | 267 | 44.494 | 23.163 | 22.728 | 1.00 | 21.76 | C |
| ATOM | 3846 | CD2 | PHE | B | 267 | 43.528 | 22.280 | 23.208 | 1.00 | 22.15 | C |
| ATOM | 3847 | N | ARG | B | 268 | 38.764 | 20.479 | 25.575 | 1.00 | 23.30 | N |
| ATOM | 3848 | CA | ARG | B | 268 | 37.503 | 19.763 | 25.764 | 1.00 | 23.41 | C |
| ATOM | 3849 | C | ARG | B | 268 | 36.434 | 20.675 | 26.377 | 1.00 | 23.37 | C |
| ATOM | 3850 | O | ARG | B | 268 | 35.277 | 20.652 | 25.955 | 1.00 | 23.33 | O |
| ATOM | 3851 | CB | ARG | B | 268 | 37.712 | 18.516 | 26.629 | 1.00 | 23.25 | C |
| ATOM | 3852 | N | GLU | B | 269 | 36.837 | 21.479 | 27.362 | 1.00 | 23.40 | N |
| ATOM | 3853 | CA | GLU | B | 269 | 35.951 | 22.461 | 27.993 | 1.00 | 23.39 | C |
| ATOM | 3854 | C | GLU | B | 269 | 35.597 | 23.593 | 27.031 | 1.00 | 23.21 | C |
| ATOM | 3855 | O | GLU | B | 269 | 34.508 | 24.163 | 27.107 | 1.00 | 23.24 | O |
| ATOM | 3856 | CB | GLU | B | 269 | 36.597 | 23.045 | 29.251 | 1.00 | 23.52 | C |
| ATOM | 3857 | CG | GLU | B | 269 | 36.686 | 22.083 | 30.427 | 1.00 | 23.83 | C |
| ATOM | 3858 | CD | GLU | B | 269 | 37.748 | 22.483 | 31.438 | 1.00 | 24.73 | C |
| ATOM | 3859 | OE1 | GLU | B | 269 | 38.548 | 23.402 | 31.149 | 1.00 | 25.10 | O |
| ATOM | 3860 | OE2 | GLU | B | 269 | 37.783 | 21.878 | 32.531 | 1.00 | 25.14 | O |
| ATOM | 3861 | N | LEU | B | 270 | 36.527 | 23.908 | 26.133 | 1.00 | 23.07 | N |
| ATOM | 3862 | CA | LEU | B | 270 | 36.321 | 24.933 | 25.114 | 1.00 | 22.76 | C |
| ATOM | 3863 | C | LEU | B | 270 | 35.275 | 24.523 | 24.075 | 1.00 | 22.71 | C |
| ATOM | 3864 | O | LEU | B | 270 | 34.531 | 25.369 | 23.577 | 1.00 | 22.69 | O |
| ATOM | 3865 | CB | LEU | B | 270 | 37.649 | 25.288 | 24.433 | 1.00 | 22.70 | C |
| ATOM | 3866 | CG | LEU | B | 270 | 38.618 | 26.170 | 25.229 | 1.00 | 22.46 | C |
| ATOM | 3867 | CD1 | LEU | B | 270 | 40.030 | 26.069 | 24.672 | 1.00 | 22.28 | C |
| ATOM | 3868 | CD2 | LEU | B | 270 | 38.159 | 27.615 | 25.245 | 1.00 | 22.09 | C |
| ATOM | 3869 | N | ILE | B | 271 | 35.225 | 23.230 | 23.750 | 1.00 | 22.59 | N |
| ATOM | 3870 | CA | ILE | B | 271 | 34.211 | 22.702 | 22.835 | 1.00 | 22.57 | C |
| ATOM | 3871 | C | ILE | B | 271 | 32.812 | 22.885 | 23.422 | 1.00 | 22.61 | C |
| ATOM | 3872 | O | ILE | B | 271 | 31.893 | 23.305 | 22.720 | 1.00 | 22.45 | O |
| ATOM | 3873 | CB | ILE | B | 271 | 34.462 | 21.202 | 22.514 | 1.00 | 22.54 | C |
| ATOM | 3874 | CG1 | ILE | B | 271 | 35.747 | 21.021 | 21.706 | 1.00 | 22.32 | C |
| ATOM | 3875 | CD1 | ILE | B | 271 | 36.329 | 19.621 | 21.789 | 1.00 | 21.94 | C |
| ATOM | 3876 | CG2 | ILE | B | 271 | 33.276 | 20.592 | 21.757 | 1.00 | 22.48 | C |
| ATOM | 3877 | N | ILE | B | 272 | 32.669 | 22.575 | 24.710 | 1.00 | 22.76 | N |
| ATOM | 3878 | CA | ILE | B | 272 | 31.377 | 22.631 | 25.396 | 1.00 | 22.92 | C |
| ATOM | 3879 | C | ILE | B | 272 | 30.822 | 24.053 | 25.461 | 1.00 | 23.12 | C |
| ATOM | 3880 | O | ILE | B | 272 | 29.682 | 24.295 | 25.055 | 1.00 | 23.21 | O |
| ATOM | 3881 | CB | ILE | B | 272 | 31.468 | 22.006 | 26.819 | 1.00 | 22.82 | C |
| ATOM | 3882 | CG1 | ILE | B | 272 | 31.923 | 20.543 | 26.743 | 1.00 | 22.59 | C |
| ATOM | 3883 | CD1 | ILE | B | 272 | 32.685 | 20.065 | 27.961 | 1.00 | 21.74 | C |
| ATOM | 3884 | CG2 | ILE | B | 272 | 30.129 | 22.098 | 27.538 | 1.00 | 22.80 | C |
| ATOM | 3885 | N | GLU | B | 273 | 31.633 | 24.986 | 25.956 | 1.00 | 23.34 | N |
| ATOM | 3886 | CA | GLU | B | 273 | 31.180 | 26.355 | 26.192 | 1.00 | 23.79 | C |
| ATOM | 3887 | C | GLU | B | 273 | 30.864 | 27.118 | 24.906 | 1.00 | 23.85 | C |
| ATOM | 3888 | O | GLU | B | 273 | 29.939 | 27.931 | 24.877 | 1.00 | 23.84 | O |
| ATOM | 3889 | CB | GLU | B | 273 | 32.190 | 27.123 | 27.049 | 1.00 | 24.01 | C |
| ATOM | 3890 | CG | GLU | B | 273 | 31.702 | 27.421 | 28.464 | 1.00 | 24.72 | C |
| ATOM | 3891 | CD | GLU | B | 273 | 31.395 | 26.165 | 29.265 | 1.00 | 25.33 | C |
| ATOM | 3892 | OE1 | GLU | B | 273 | 32.345 | 25.518 | 29.760 | 1.00 | 25.88 | O |
| ATOM | 3893 | OE2 | GLU | B | 273 | 30.202 | 25.819 | 29.397 | 1.00 | 25.43 | O |
| ATOM | 3894 | N | PHE | B | 274 | 31.624 | 26.848 | 23.849 | 1.00 | 23.85 | N |
| ATOM | 3895 | CA | PHE | B | 274 | 31.379 | 27.482 | 22.559 | 1.00 | 23.81 | C |

FIG. 4MMM

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3896 | C | PHE | B | 274 | 30.189 | 26.858 | 21.835 | 1.00 | 24.11 | C |
| ATOM | 3897 | O | PHE | B | 274 | 29.513 | 27.531 | 21.056 | 1.00 | 24.18 | O |
| ATOM | 3898 | CB | PHE | B | 274 | 32.634 | 27.463 | 21.685 | 1.00 | 23.47 | C |
| ATOM | 3899 | CG | PHE | B | 274 | 33.524 | 28.661 | 21.880 | 1.00 | 22.83 | C |
| ATOM | 3900 | CD1 | PHE | B | 274 | 33.143 | 29.915 | 21.407 | 1.00 | 22.33 | C |
| ATOM | 3901 | CE1 | PHE | B | 274 | 33.962 | 31.027 | 21.586 | 1.00 | 21.86 | C |
| ATOM | 3902 | CZ | PHE | B | 274 | 35.178 | 30.891 | 22.247 | 1.00 | 21.83 | C |
| ATOM | 3903 | CE2 | PHE | B | 274 | 35.567 | 29.643 | 22.726 | 1.00 | 22.15 | C |
| ATOM | 3904 | CD2 | PHE | B | 274 | 34.740 | 28.537 | 22.541 | 1.00 | 22.25 | C |
| ATOM | 3905 | N | SER | B | 275 | 29.937 | 25.576 | 22.100 | 1.00 | 24.38 | N |
| ATOM | 3906 | CA | SER | B | 275 | 28.752 | 24.892 | 21.589 | 1.00 | 24.77 | C |
| ATOM | 3907 | C | SER | B | 275 | 27.493 | 25.446 | 22.243 | 1.00 | 25.16 | C |
| ATOM | 3908 | O | SER | B | 275 | 26.458 | 25.592 | 21.589 | 1.00 | 25.23 | O |
| ATOM | 3909 | CB | SER | B | 275 | 28.841 | 23.386 | 21.840 | 1.00 | 24.72 | C |
| ATOM | 3910 | OG | SER | B | 275 | 29.854 | 22.793 | 21.046 | 1.00 | 25.10 | O |
| ATOM | 3911 | N | LYS | B | 276 | 27.595 | 25.742 | 23.538 | 1.00 | 25.66 | N |
| ATOM | 3912 | CA | LYS | B | 276 | 26.512 | 26.348 | 24.304 | 1.00 | 26.04 | C |
| ATOM | 3913 | C | LYS | B | 276 | 26.185 | 27.730 | 23.745 | 1.00 | 26.35 | C |
| ATOM | 3914 | O | LYS | B | 276 | 25.018 | 28.110 | 23.652 | 1.00 | 26.43 | O |
| ATOM | 3915 | CB | LYS | B | 276 | 26.901 | 26.446 | 25.782 | 1.00 | 26.03 | C |
| ATOM | 3916 | CG | LYS | B | 276 | 25.763 | 26.832 | 26.715 | 1.00 | 25.87 | C |
| ATOM | 3917 | N | MET | B | 277 | 27.228 | 28.465 | 23.368 | 1.00 | 26.84 | N |
| ATOM | 3918 | CA | MET | B | 277 | 27.082 | 29.782 | 22.756 | 1.00 | 27.25 | C |
| ATOM | 3919 | C | MET | B | 277 | 26.618 | 29.679 | 21.302 | 1.00 | 27.53 | C |
| ATOM | 3920 | O | MET | B | 277 | 25.908 | 30.553 | 20.814 | 1.00 | 27.62 | O |
| ATOM | 3921 | CB | MET | B | 277 | 28.391 | 30.570 | 22.855 | 1.00 | 27.16 | C |
| ATOM | 3922 | CG | MET | B | 277 | 28.783 | 30.929 | 24.282 | 1.00 | 27.12 | C |
| ATOM | 3923 | SD | MET | B | 277 | 30.441 | 31.625 | 24.421 | 1.00 | 27.75 | S |
| ATOM | 3924 | CE | MET | B | 277 | 30.391 | 32.243 | 26.081 | 1.00 | 27.55 | C |
| ATOM | 3925 | N | ALA | B | 278 | 27.011 | 28.601 | 20.626 | 1.00 | 28.12 | N |
| ATOM | 3926 | CA | ALA | B | 278 | 26.583 | 28.336 | 19.250 | 1.00 | 28.73 | C |
| ATOM | 3927 | C | ALA | B | 278 | 25.097 | 27.981 | 19.163 | 1.00 | 29.23 | C |
| ATOM | 3928 | O | ALA | B | 278 | 24.518 | 27.967 | 18.073 | 1.00 | 29.49 | O |
| ATOM | 3929 | CB | ALA | B | 278 | 27.428 | 27.230 | 18.634 | 1.00 | 28.63 | C |
| ATOM | 3930 | N | ARG | B | 279 | 24.493 | 27.695 | 20.314 | 1.00 | 29.77 | N |
| ATOM | 3931 | CA | ARG | B | 279 | 23.075 | 27.360 | 20.398 | 1.00 | 30.15 | C |
| ATOM | 3932 | C | ARG | B | 279 | 22.201 | 28.612 | 20.394 | 1.00 | 30.30 | C |
| ATOM | 3933 | O | ARG | B | 279 | 21.026 | 28.556 | 20.029 | 1.00 | 30.44 | O |
| ATOM | 3934 | CB | ARG | B | 279 | 22.806 | 26.539 | 21.659 | 1.00 | 30.29 | C |
| ATOM | 3935 | CG | ARG | B | 279 | 22.364 | 25.110 | 21.394 | 1.00 | 30.93 | C |
| ATOM | 3936 | CD | ARG | B | 279 | 23.462 | 24.072 | 21.569 | 1.00 | 31.45 | C |
| ATOM | 3937 | NE | ARG | B | 279 | 23.708 | 23.750 | 22.975 | 1.00 | 31.80 | N |
| ATOM | 3938 | CZ | ARG | B | 279 | 24.647 | 22.910 | 23.403 | 1.00 | 32.04 | C |
| ATOM | 3939 | NH1 | ARG | B | 279 | 24.792 | 22.686 | 24.703 | 1.00 | 32.21 | N |
| ATOM | 3940 | NH2 | ARG | B | 279 | 25.444 | 22.290 | 22.539 | 1.00 | 31.88 | N |
| ATOM | 3941 | N | ASP | B | 280 | 22.785 | 29.734 | 20.805 | 1.00 | 30.56 | N |
| ATOM | 3942 | CA | ASP | B | 280 | 22.081 | 31.010 | 20.904 | 1.00 | 30.76 | C |
| ATOM | 3943 | C | ASP | B | 280 | 23.089 | 32.142 | 20.663 | 1.00 | 30.85 | C |
| ATOM | 3944 | O | ASP | B | 280 | 23.477 | 32.846 | 21.600 | 1.00 | 30.94 | O |
| ATOM | 3945 | CB | ASP | B | 280 | 21.418 | 31.130 | 22.284 | 1.00 | 30.99 | C |
| ATOM | 3946 | CG | ASP | B | 280 | 20.542 | 32.370 | 22.426 | 1.00 | 31.58 | C |
| ATOM | 3947 | OD1 | ASP | B | 280 | 20.137 | 32.963 | 21.401 | 1.00 | 32.09 | O |
| ATOM | 3948 | OD2 | ASP | B | 280 | 20.204 | 32.819 | 23.542 | 1.00 | 31.92 | O |
| ATOM | 3949 | N | PRO | B | 281 | 23.509 | 32.313 | 19.406 | 1.00 | 30.83 | N |
| ATOM | 3950 | CA | PRO | B | 281 | 24.641 | 33.191 | 19.071 | 1.00 | 30.79 | C |
| ATOM | 3951 | C | PRO | B | 281 | 24.399 | 34.683 | 19.311 | 1.00 | 30.73 | C |
| ATOM | 3952 | O | PRO | B | 281 | 25.361 | 35.416 | 19.558 | 1.00 | 30.61 | O |
| ATOM | 3953 | CB | PRO | B | 281 | 24.864 | 32.919 | 17.580 | 1.00 | 30.83 | C |
| ATOM | 3954 | CG | PRO | B | 281 | 23.553 | 32.440 | 17.078 | 1.00 | 30.89 | C |
| ATOM | 3955 | CD | PRO | B | 281 | 22.931 | 31.681 | 18.205 | 1.00 | 30.85 | C |

FIG. 4NNN

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3956 | N | GLN | B | 282 | 23.143 | 35.115 | 19.244 | 1.00 | 30.74 | N |
| ATOM | 3957 | CA | GLN | B | 282 | 22.789 | 36.524 | 19.422 | 1.00 | 30.84 | C |
| ATOM | 3958 | C | GLN | B | 282 | 23.001 | 36.998 | 20.861 | 1.00 | 30.75 | C |
| ATOM | 3959 | O | GLN | B | 282 | 23.153 | 38.194 | 21.114 | 1.00 | 30.84 | O |
| ATOM | 3960 | CB | GLN | B | 282 | 21.340 | 36.774 | 18.992 | 1.00 | 30.99 | C |
| ATOM | 3961 | CG | GLN | B | 282 | 20.970 | 36.173 | 17.635 | 1.00 | 31.18 | C |
| ATOM | 3962 | CD | GLN | B | 282 | 20.824 | 37.215 | 16.543 | 1.00 | 31.13 | C |
| ATOM | 3963 | OE1 | GLN | B | 282 | 20.420 | 38.347 | 16.805 | 1.00 | 31.87 | O |
| ATOM | 3964 | NE2 | GLN | B | 282 | 21.143 | 36.832 | 15.314 | 1.00 | 31.11 | N |
| ATOM | 3965 | N | ARG | B | 283 | 23.015 | 36.047 | 21.791 | 1.00 | 30.72 | N |
| ATOM | 3966 | CA | ARG | B | 283 | 23.224 | 36.327 | 23.206 | 1.00 | 30.66 | C |
| ATOM | 3967 | C | ARG | B | 283 | 24.686 | 36.632 | 23.523 | 1.00 | 30.48 | C |
| ATOM | 3968 | O | ARG | B | 283 | 24.986 | 37.264 | 24.538 | 1.00 | 30.68 | O |
| ATOM | 3969 | CB | ARG | B | 283 | 22.751 | 35.137 | 24.049 | 1.00 | 30.76 | C |
| ATOM | 3970 | CG | ARG | B | 283 | 22.352 | 35.492 | 25.476 | 1.00 | 31.39 | C |
| ATOM | 3971 | CD | ARG | B | 283 | 21.641 | 34.373 | 26.224 | 1.00 | 32.24 | C |
| ATOM | 3972 | NE | ARG | B | 283 | 22.182 | 34.181 | 27.570 | 1.00 | 32.93 | N |
| ATOM | 3973 | CZ | ARG | B | 283 | 21.462 | 33.846 | 28.638 | 1.00 | 33.23 | C |
| ATOM | 3974 | NH1 | ARG | B | 283 | 22.059 | 33.695 | 29.814 | 1.00 | 33.09 | N |
| ATOM | 3975 | NH2 | ARG | B | 283 | 20.149 | 33.658 | 28.541 | 1.00 | 33.41 | N |
| ATOM | 3976 | N | TYR | B | 284 | 25.591 | 36.190 | 22.654 | 1.00 | 30.20 | N |
| ATOM | 3977 | CA | TYR | B | 284 | 27.020 | 36.234 | 22.957 | 1.00 | 29.92 | C |
| ATOM | 3978 | C | TYR | B | 284 | 27.840 | 37.084 | 21.988 | 1.00 | 29.85 | C |
| ATOM | 3979 | O | TYR | B | 284 | 28.956 | 37.494 | 22.313 | 1.00 | 29.72 | O |
| ATOM | 3980 | CB | TYR | B | 284 | 27.583 | 34.812 | 23.069 | 1.00 | 29.87 | C |
| ATOM | 3981 | CG | TYR | B | 284 | 26.868 | 33.973 | 24.108 | 1.00 | 29.73 | C |
| ATOM | 3982 | CD1 | TYR | B | 284 | 25.850 | 33.094 | 23.742 | 1.00 | 29.75 | C |
| ATOM | 3983 | CE1 | TYR | B | 284 | 25.184 | 32.327 | 24.695 | 1.00 | 29.98 | C |
| ATOM | 3984 | CZ | TYR | B | 284 | 25.535 | 32.443 | 26.032 | 1.00 | 29.92 | C |
| ATOM | 3985 | OH | TYR | B | 284 | 24.883 | 31.690 | 26.983 | 1.00 | 29.95 | O |
| ATOM | 3986 | CE2 | TYR | B | 284 | 26.541 | 33.311 | 26.418 | 1.00 | 29.77 | C |
| ATOM | 3987 | CD2 | TYR | B | 284 | 27.199 | 34.071 | 25.458 | 1.00 | 29.72 | C |
| ATOM | 3988 | N | LEU | B | 285 | 27.285 | 37.352 | 20.807 | 1.00 | 29.69 | N |
| ATOM | 3989 | CA | LEU | B | 285 | 27.907 | 38.272 | 19.856 | 1.00 | 29.64 | C |
| ATOM | 3990 | C | LEU | B | 285 | 26.898 | 39.279 | 19.302 | 1.00 | 29.82 | C |
| ATOM | 3991 | O | LEU | B | 285 | 25.762 | 38.920 | 18.971 | 1.00 | 29.58 | O |
| ATOM | 3992 | CB | LEU | B | 285 | 28.593 | 37.513 | 18.714 | 1.00 | 29.47 | C |
| ATOM | 3993 | CG | LEU | B | 285 | 29.794 | 36.606 | 19.007 | 1.00 | 28.85 | C |
| ATOM | 3994 | CD1 | LEU | B | 285 | 30.244 | 35.920 | 17.730 | 1.00 | 28.51 | C |
| ATOM | 3995 | CD2 | LEU | B | 285 | 30.950 | 37.368 | 19.639 | 1.00 | 28.37 | C |
| ATOM | 3996 | N | VAL | B | 286 | 27.323 | 40.539 | 19.209 | 1.00 | 29.96 | N |
| ATOM | 3997 | CA | VAL | B | 286 | 26.472 | 41.622 | 18.716 | 1.00 | 30.20 | C |
| ATOM | 3998 | C | VAL | B | 286 | 27.058 | 42.233 | 17.440 | 1.00 | 30.44 | C |
| ATOM | 3999 | O | VAL | B | 286 | 28.050 | 42.968 | 17.485 | 1.00 | 30.62 | O |
| ATOM | 4000 | CB | VAL | B | 286 | 26.249 | 42.726 | 19.793 | 1.00 | 30.23 | C |
| ATOM | 4001 | CG1 | VAL | B | 286 | 25.298 | 43.807 | 19.284 | 1.00 | 30.11 | C |
| ATOM | 4002 | CG2 | VAL | B | 286 | 25.725 | 42.125 | 21.095 | 1.00 | 30.10 | C |
| ATOM | 4003 | N | ILE | B | 287 | 26.442 | 41.912 | 16.306 | 1.00 | 30.62 | N |
| ATOM | 4004 | CA | ILE | B | 287 | 26.855 | 42.455 | 15.013 | 1.00 | 30.93 | C |
| ATOM | 4005 | C | ILE | B | 287 | 25.692 | 43.218 | 14.381 | 1.00 | 31.07 | C |
| ATOM | 4006 | O | ILE | B | 287 | 24.540 | 42.781 | 14.454 | 1.00 | 31.00 | O |
| ATOM | 4007 | CB | ILE | B | 287 | 27.372 | 41.330 | 14.065 | 1.00 | 31.02 | C |
| ATOM | 4008 | CG1 | ILE | B | 287 | 28.484 | 40.514 | 14.734 | 1.00 | 30.90 | C |
| ATOM | 4009 | CD1 | ILE | B | 287 | 28.421 | 39.033 | 14.443 | 1.00 | 31.01 | C |
| ATOM | 4010 | CG2 | ILE | B | 287 | 27.888 | 41.917 | 12.749 | 1.00 | 31.03 | C |
| ATOM | 4011 | N | GLN | B | 288 | 26.004 | 44.363 | 13.775 | 1.00 | 31.11 | N |
| ATOM | 4012 | CA | GLN | B | 288 | 25.006 | 45.206 | 13.117 | 1.00 | 30.91 | C |
| ATOM | 4013 | C | GLN | B | 288 | 24.328 | 44.472 | 11.961 | 1.00 | 30.82 | C |
| ATOM | 4014 | O | GLN | B | 288 | 23.103 | 44.524 | 11.817 | 1.00 | 30.96 | O |
| ATOM | 4015 | CB | GLN | B | 288 | 25.647 | 46.504 | 12.620 | 1.00 | 31.04 | C |

FIG. 4000

| | | | | | | | | | | | |
|--------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 4016 | N | GLY | B | 289 | 25.130 | 43.781 | 11.151 | 1.00 | 30.32 | N |
| ATOM | 4017 | CA | GLY | B | 289 | 24.620 | 42.982 | 10.050 | 1.00 | 29.97 | C |
| ATOM | 4018 | C | GLY | B | 289 | 24.025 | 41.663 | 10.514 | 1.00 | 29.71 | C |
| ATOM | 4019 | O | GLY | B | 289 | 24.322 | 40.603 | 9.951 | 1.00 | 29.80 | O |
| ATOM | 4020 | N | GLU | B | 290 | 23.179 | 41.739 | 11.540 | 1.00 | 29.17 | N |
| ATOM | 4021 | CA | GLU | B | 290 | 22.544 | 40.570 | 12.140 | 1.00 | 28.68 | C |
| ATOM | 4022 | C | GLU | B | 290 | 21.102 | 40.887 | 12.531 | 1.00 | 28.79 | C |
| ATOM | 4023 | O | GLU | B | 290 | 20.511 | 41.853 | 12.040 | 1.00 | 28.90 | O |
| ATOM | 4024 | CB | GLU | B | 290 | 23.334 | 40.116 | 13.372 | 1.00 | 28.31 | C |
| ATOM | 4025 | CG | GLU | B | 290 | 23.386 | 38.610 | 13.587 | 1.00 | 27.52 | C |
| ATOM | 4026 | CD | GLU | B | 290 | 24.270 | 37.885 | 12.588 | 1.00 | 27.08 | C |
| ATOM | 4027 | OE1 | GLU | B | 290 | 25.146 | 38.521 | 11.963 | 1.00 | 27.14 | O |
| ATOM | 4028 | OE2 | GLU | B | 290 | 24.084 | 36.665 | 12.425 | 1.00 | 27.57 | O |
| TER | 4029 | | GLU | B | 290 | | | | | | |
| HETATM | 4030 | O1A | ANP | W | 1 | 54.152 | 28.767 | 4.525 | 1.00 | 14.19 | O |
| HETATM | 4031 | PA | ANP | W | 1 | 52.665 | 29.162 | 4.909 | 1.00 | 14.23 | P |
| HETATM | 4032 | O2A | ANP | W | 1 | 52.045 | 28.041 | 5.844 | 1.00 | 14.69 | O |
| HETATM | 4033 | O3A | ANP | W | 1 | 52.635 | 30.626 | 5.591 | 1.00 | 14.46 | O |
| HETATM | 4034 | PB | ANP | W | 1 | 51.592 | 31.138 | 6.713 | 1.00 | 14.01 | P |
| HETATM | 4035 | O1B | ANP | W | 1 | 50.427 | 30.096 | 6.982 | 1.00 | 14.07 | O |
| HETATM | 4036 | O2B | ANP | W | 1 | 50.966 | 32.525 | 6.257 | 1.00 | 14.38 | O |
| HETATM | 4037 | N3B | ANP | W | 1 | 52.464 | 31.438 | 8.189 | 1.00 | 13.82 | N |
| HETATM | 4038 | PG | ANP | W | 1 | 53.106 | 30.114 | 9.118 | 1.00 | 12.66 | P |
| HETATM | 4039 | O3G | ANP | W | 1 | 52.248 | 28.804 | 8.839 | 1.00 | 13.65 | O |
| HETATM | 4040 | O2G | ANP | W | 1 | 53.031 | 30.526 | 10.647 | 1.00 | 13.04 | O |
| HETATM | 4041 | O1G | ANP | W | 1 | 54.615 | 29.839 | 8.717 | 1.00 | 12.98 | O |
| HETATM | 4042 | O5* | ANP | W | 1 | 51.775 | 29.328 | 3.577 | 1.00 | 15.00 | O |
| HETATM | 4043 | C5* | ANP | W | 1 | 51.932 | 30.426 | 2.677 | 1.00 | 15.96 | C |
| HETATM | 4044 | C4* | ANP | W | 1 | 50.621 | 30.671 | 1.929 | 1.00 | 16.58 | C |
| HETATM | 4045 | O4* | ANP | W | 1 | 50.160 | 29.456 | 1.323 | 1.00 | 16.78 | O |
| HETATM | 4046 | C1* | ANP | W | 1 | 48.800 | 29.196 | 1.685 | 1.00 | 17.15 | C |
| HETATM | 4047 | C2* | ANP | W | 1 | 48.549 | 29.985 | 2.965 | 1.00 | 17.11 | C |
| HETATM | 4048 | O2* | ANP | W | 1 | 47.198 | 30.414 | 3.085 | 1.00 | 16.97 | O |
| HETATM | 4049 | C3* | ANP | W | 1 | 49.514 | 31.155 | 2.857 | 1.00 | 16.74 | C |
| HETATM | 4050 | O3* | ANP | W | 1 | 48.868 | 32.271 | 2.273 | 1.00 | 16.57 | O |
| HETATM | 4051 | N9 | ANP | W | 1 | 48.587 | 27.743 | 1.894 | 1.00 | 17.64 | N |
| HETATM | 4052 | C8 | ANP | W | 1 | 49.262 | 26.916 | 2.735 | 1.00 | 17.81 | C |
| HETATM | 4053 | N7 | ANP | W | 1 | 48.810 | 25.620 | 2.687 | 1.00 | 18.02 | N |
| HETATM | 4054 | C5 | ANP | W | 1 | 47.812 | 25.599 | 1.786 | 1.00 | 18.38 | C |
| HETATM | 4055 | C6 | ANP | W | 1 | 46.850 | 24.636 | 1.180 | 1.00 | 18.92 | C |
| HETATM | 4056 | N6 | ANP | W | 1 | 46.865 | 23.332 | 1.554 | 1.00 | 19.07 | N |
| HETATM | 4057 | C4 | ANP | W | 1 | 47.693 | 26.965 | 1.301 | 1.00 | 17.99 | C |
| HETATM | 4058 | N3 | ANP | W | 1 | 46.710 | 27.322 | 0.309 | 1.00 | 18.03 | N |
| HETATM | 4059 | C2 | ANP | W | 1 | 45.899 | 26.361 | -0.165 | 1.00 | 18.44 | C |
| HETATM | 4060 | N1 | ANP | W | 1 | 45.961 | 25.077 | 0.249 | 1.00 | 18.87 | N |
| HETATM | 4061 | O1A | ANP | W | 2 | 19.403 | 6.203 | 15.674 | 1.00 | 15.26 | O |
| HETATM | 4062 | PA | ANP | W | 2 | 18.049 | 5.565 | 16.209 | 1.00 | 15.32 | P |
| HETATM | 4063 | O2A | ANP | W | 2 | 18.326 | 4.676 | 17.493 | 1.00 | 15.23 | O |
| HETATM | 4064 | O3A | ANP | W | 2 | 16.971 | 6.730 | 16.499 | 1.00 | 15.88 | O |
| HETATM | 4065 | PB | ANP | W | 2 | 15.646 | 6.537 | 17.396 | 1.00 | 16.01 | P |
| HETATM | 4066 | O1B | ANP | W | 2 | 15.547 | 5.062 | 17.973 | 1.00 | 16.94 | O |
| HETATM | 4067 | O2B | ANP | W | 2 | 14.364 | 6.863 | 16.519 | 1.00 | 16.42 | O |
| HETATM | 4068 | N3B | ANP | W | 2 | 15.695 | 7.656 | 18.730 | 1.00 | 16.44 | N |
| HETATM | 4069 | PG | ANP | W | 2 | 16.958 | 7.503 | 19.920 | 1.00 | 16.23 | P |
| HETATM | 4070 | O3G | ANP | W | 2 | 17.525 | 6.020 | 19.897 | 1.00 | 16.82 | O |
| HETATM | 4071 | O2G | ANP | W | 2 | 16.321 | 7.826 | 21.340 | 1.00 | 16.56 | O |
| HETATM | 4072 | O1G | ANP | W | 2 | 18.143 | 8.515 | 19.599 | 1.00 | 16.37 | O |
| HETATM | 4073 | O5* | ANP | W | 2 | 17.363 | 4.666 | 15.069 | 1.00 | 15.30 | O |
| HETATM | 4074 | C5* | ANP | W | 2 | 16.957 | 5.226 | 13.824 | 1.00 | 15.80 | C |
| HETATM | 4075 | C4* | ANP | W | 2 | 16.040 | 4.244 | 13.108 | 1.00 | 16.07 | C |

FIG. 4PPP

| | | | | | | | | | | | |
|--------|------|-----|-----|---|----|---------|---------|--------|------|-------|----|
| HETATM | 4076 | O4* | ANP | W | 2 | 16.717 | 2.997 | 12.922 | 1.00 | 16.33 | O |
| HETATM | 4077 | C1* | ANP | W | 2 | 15.922 | 1.921 | 13.431 | 1.00 | 16.41 | C |
| HETATM | 4078 | C2* | ANP | W | 2 | 14.972 | 2.540 | 14.445 | 1.00 | 16.48 | C |
| HETATM | 4079 | O2* | ANP | W | 2 | 13.732 | 1.854 | 14.511 | 1.00 | 16.84 | O |
| HETATM | 4080 | C3* | ANP | W | 2 | 14.786 | 3.951 | 13.916 | 1.00 | 16.27 | C |
| HETATM | 4081 | O3* | ANP | W | 2 | 13.667 | 4.004 | 13.048 | 1.00 | 16.31 | O |
| HETATM | 4082 | N9 | ANP | W | 2 | 16.810 | 0.874 | 13.995 | 1.00 | 16.25 | N |
| HETATM | 4083 | C8 | ANP | W | 2 | 17.822 | 1.016 | 14.888 | 1.00 | 16.35 | C |
| HETATM | 4084 | N7 | ANP | W | 2 | 18.453 | -0.174 | 15.174 | 1.00 | 16.50 | N |
| HETATM | 4085 | C5 | ANP | W | 2 | 17.839 | -1.115 | 14.436 | 1.00 | 16.63 | C |
| HETATM | 4086 | C6 | ANP | W | 2 | 17.907 | -2.578 | 14.172 | 1.00 | 16.77 | C |
| HETATM | 4087 | N6 | ANP | W | 2 | 18.829 | -3.340 | 14.806 | 1.00 | 17.13 | N |
| HETATM | 4088 | C4 | ANP | W | 2 | 16.800 | -0.416 | 13.694 | 1.00 | 16.65 | C |
| HETATM | 4089 | N3 | ANP | W | 2 | 15.924 | -1.117 | 12.781 | 1.00 | 16.77 | N |
| HETATM | 4090 | C2 | ANP | W | 2 | 16.087 | -2.445 | 12.630 | 1.00 | 16.80 | C |
| HETATM | 4091 | N1 | ANP | W | 2 | 17.035 | -3.143 | 13.293 | 1.00 | 16.71 | N |
| HETATM | 4092 | MG | MG | W | 3 | 50.504 | 28.210 | 7.268 | 1.00 | 25.98 | MG |
| HETATM | 4093 | MG | MG | W | 4 | 16.970 | 3.922 | 18.643 | 1.00 | 7.82 | MG |
| HETATM | 4094 | O | HOH | W | 5 | 4.290 | 11.548 | 33.626 | 1.00 | 6.42 | O |
| HETATM | 4095 | O | HOH | W | 6 | 18.999 | -0.021 | 34.227 | 1.00 | 16.10 | O |
| HETATM | 4096 | O | HOH | W | 7 | 50.184 | 27.299 | 18.765 | 1.00 | 3.07 | O |
| HETATM | 4097 | O | HOH | W | 8 | 16.094 | 5.310 | 30.267 | 1.00 | 2.00 | O |
| HETATM | 4098 | O | HOH | W | 9 | 21.140 | -9.281 | 11.284 | 1.00 | 13.72 | O |
| HETATM | 4099 | O | HOH | W | 10 | 12.663 | -11.281 | 13.567 | 1.00 | 30.98 | O |
| HETATM | 4100 | O | HOH | W | 11 | 42.871 | 16.268 | 5.531 | 1.00 | 3.37 | O |
| HETATM | 4101 | O | HOH | W | 12 | 5.321 | 8.123 | 21.448 | 1.00 | 13.81 | O |
| HETATM | 4102 | O | HOH | W | 13 | 12.492 | -7.983 | 13.744 | 1.00 | 17.68 | O |
| HETATM | 4103 | O | HOH | W | 14 | -10.354 | -6.119 | 27.605 | 1.00 | 32.05 | O |
| HETATM | 4104 | O | HOH | W | 15 | 44.859 | 36.969 | 30.762 | 1.00 | 6.38 | O |
| HETATM | 4105 | O | HOH | W | 16 | -10.333 | 1.111 | 37.170 | 1.00 | 40.24 | O |
| HETATM | 4106 | O | HOH | W | 17 | 15.243 | -4.807 | 39.557 | 1.00 | 5.14 | O |
| HETATM | 4107 | O | HOH | W | 18 | 28.726 | -6.171 | 34.736 | 1.00 | 11.86 | O |
| HETATM | 4108 | O | HOH | W | 19 | 30.980 | 44.276 | 27.536 | 1.00 | 5.15 | O |
| HETATM | 4109 | O | HOH | W | 20 | 44.582 | 32.439 | 1.893 | 1.00 | 13.93 | O |
| HETATM | 4110 | O | HOH | W | 21 | 40.070 | 32.836 | 2.334 | 1.00 | 2.00 | O |
| HETATM | 4111 | O | HOH | W | 22 | 41.231 | 18.825 | 25.667 | 1.00 | 10.34 | O |
| HETATM | 4112 | O | HOH | W | 23 | 52.638 | 29.706 | 18.724 | 1.00 | 44.04 | O |
| HETATM | 4113 | O | HOH | W | 24 | 34.149 | -9.405 | 10.655 | 1.00 | 28.63 | O |
| HETATM | 4114 | O | HOH | W | 25 | -5.908 | 11.084 | 33.794 | 1.00 | 20.58 | O |
| HETATM | 4115 | O | HOH | W | 26 | 21.006 | 20.012 | 31.996 | 1.00 | 24.85 | O |
| HETATM | 4116 | O | HOH | W | 27 | 52.463 | 34.089 | 4.899 | 1.00 | 20.21 | O |
| HETATM | 4117 | O | HOH | W | 28 | 11.154 | -10.162 | 43.370 | 1.00 | 21.83 | O |
| HETATM | 4118 | O | HOH | W | 29 | 14.409 | 8.134 | 26.716 | 1.00 | 26.10 | O |
| HETATM | 4119 | O | HOH | W | 30 | 48.209 | 9.659 | 1.939 | 1.00 | 33.23 | O |
| HETATM | 4120 | O | HOH | W | 31 | 6.904 | -1.951 | 13.417 | 1.00 | 25.25 | O |
| HETATM | 4121 | O | HOH | W | 32 | 15.899 | -10.068 | 34.616 | 1.00 | 4.64 | O |
| HETATM | 4122 | O | HOH | W | 33 | 47.779 | 20.359 | 21.519 | 1.00 | 5.98 | O |
| HETATM | 4123 | O | HOH | W | 34 | 3.700 | 10.587 | 40.253 | 1.00 | 7.89 | O |
| HETATM | 4124 | O | HOH | W | 35 | -11.781 | -7.560 | 24.631 | 1.00 | 26.81 | O |
| HETATM | 4125 | O | HOH | W | 36 | 37.071 | 47.600 | 22.181 | 1.00 | 31.63 | O |
| HETATM | 4126 | O | HOH | W | 37 | 53.336 | 25.403 | 28.783 | 1.00 | 15.60 | O |
| HETATM | 4127 | O | HOH | W | 38 | 34.560 | -9.596 | 23.541 | 1.00 | 32.06 | O |
| HETATM | 4128 | O | HOH | W | 39 | 44.712 | 45.040 | 28.718 | 1.00 | 29.39 | O |
| HETATM | 4129 | O | HOH | W | 40 | 32.687 | 0.085 | 5.244 | 1.00 | 34.81 | O |
| HETATM | 4130 | O | HOH | W | 41 | 29.485 | -10.969 | 17.606 | 1.00 | 24.11 | O |
| HETATM | 4131 | O | HOH | W | 42 | 55.740 | 27.886 | 6.683 | 1.00 | 14.12 | O |
| HETATM | 4132 | O | HOH | W | 43 | -8.611 | -7.982 | 24.987 | 1.00 | 15.68 | O |
| HETATM | 4133 | O | HOH | W | 44 | 32.322 | -9.118 | 24.990 | 1.00 | 18.15 | O |
| HETATM | 4134 | O | HOH | W | 45 | 0.125 | 16.011 | 31.233 | 1.00 | 17.73 | O |
| HETATM | 4135 | O | HOH | W | 46 | 20.590 | 7.834 | 17.742 | 1.00 | 25.02 | O |

FIG. 4QQQ

| | | | | | | | | | | | |
|--------|------|---|-----|---|----|--------|---------|--------|------|-------|---|
| HETATM | 4136 | O | HOH | W | 47 | 49.359 | 25.038 | 5.554 | 1.00 | 13.72 | O |
| HETATM | 4137 | O | HOH | W | 48 | 34.347 | 3.367 | 11.863 | 1.00 | 13.64 | O |
| HETATM | 4138 | O | HOH | W | 49 | -1.101 | 23.372 | 37.260 | 1.00 | 25.81 | O |
| HETATM | 4139 | O | HOH | W | 50 | 45.799 | 45.166 | 19.287 | 1.00 | 25.43 | O |
| HETATM | 4140 | O | HOH | W | 51 | 25.282 | -14.857 | 30.672 | 1.00 | 22.55 | O |
| HETATM | 4141 | O | HOH | W | 52 | 52.355 | 26.732 | 21.087 | 1.00 | 23.92 | O |
| HETATM | 4142 | O | HOH | W | 53 | 43.158 | 15.435 | 26.674 | 1.00 | 32.37 | O |
| HETATM | 4143 | O | HOH | W | 54 | 34.583 | 43.175 | 16.714 | 1.00 | 25.93 | O |
| HETATM | 4144 | O | HOH | W | 55 | 38.962 | 24.995 | 0.100 | 1.00 | 25.43 | O |
| HETATM | 4145 | O | HOH | W | 56 | 42.851 | 14.558 | 9.528 | 1.00 | 24.68 | O |
| HETATM | 4146 | O | HOH | W | 57 | 3.405 | 21.917 | 22.000 | 1.00 | 20.97 | O |
| HETATM | 4147 | O | HOH | W | 58 | 23.078 | -0.069 | 19.421 | 1.00 | 19.58 | O |
| HETATM | 4148 | O | HOH | W | 59 | 14.326 | -4.757 | 6.647 | 1.00 | 19.83 | O |
| HETATM | 4149 | O | HOH | W | 60 | 28.614 | 27.321 | 1.239 | 1.00 | 27.54 | O |
| HETATM | 4150 | O | HOH | W | 61 | 48.149 | 31.411 | 5.943 | 1.00 | 14.29 | O |
| HETATM | 4151 | O | HOH | W | 62 | -0.670 | 21.642 | 39.051 | 1.00 | 22.00 | O |
| HETATM | 4152 | O | HOH | W | 63 | 24.223 | -17.815 | 26.796 | 1.00 | 23.19 | O |
| HETATM | 4153 | O | HOH | W | 64 | 43.922 | 21.892 | 26.412 | 1.00 | 27.31 | O |
| HETATM | 4154 | O | HOH | W | 65 | 15.076 | 10.275 | 18.291 | 1.00 | 26.76 | O |
| END | | | | | | | | | | | |

FIG. 4RRR

CRYST1 34.686 85.703 180.248 90.00 90.00 90.00 P 21 21 21 4

| | Atom | | | | | | | | | |
|------|------|---------|-------|----|--------|--------|--------|------|-------|------|
| | Type | Residue | # | X | Y | Z | OCC | B | | Atom |
| ATOM | 1 | N | LEU A | 9 | 8.096 | 0.008 | 38.058 | 1.00 | 35.38 | N |
| ATOM | 2 | CA | LEU A | 9 | 8.705 | -0.126 | 36.704 | 1.00 | 35.26 | C |
| ATOM | 3 | C | LEU A | 9 | 10.203 | 0.196 | 36.697 | 1.00 | 34.71 | C |
| ATOM | 4 | O | LEU A | 9 | 10.937 | -0.304 | 35.847 | 1.00 | 35.05 | O |
| ATOM | 5 | CB | LEU A | 9 | 7.966 | 0.768 | 35.699 | 1.00 | 35.55 | C |
| ATOM | 6 | CG | LEU A | 9 | 6.983 | 0.120 | 34.717 | 1.00 | 36.39 | C |
| ATOM | 7 | CD1 | LEU A | 9 | 7.718 | -0.584 | 33.591 | 1.00 | 37.01 | C |
| ATOM | 8 | CD2 | LEU A | 9 | 6.029 | -0.855 | 35.420 | 1.00 | 37.57 | C |
| ATOM | 9 | N | LEU A | 10 | 10.642 | 1.023 | 37.646 | 1.00 | 33.74 | N |
| ATOM | 10 | CA | LEU A | 10 | 12.030 | 1.475 | 37.720 | 1.00 | 32.92 | C |
| ATOM | 11 | C | LEU A | 10 | 12.862 | 0.611 | 38.659 | 1.00 | 33.05 | C |
| ATOM | 12 | O | LEU A | 10 | 12.483 | 0.374 | 39.808 | 1.00 | 32.92 | O |
| ATOM | 13 | CB | LEU A | 10 | 12.091 | 2.947 | 38.156 | 1.00 | 32.54 | C |
| ATOM | 14 | CG | LEU A | 10 | 13.449 | 3.607 | 38.424 | 1.00 | 32.04 | C |
| ATOM | 15 | CD1 | LEU A | 10 | 14.153 | 3.989 | 37.139 | 1.00 | 31.90 | C |
| ATOM | 16 | CD2 | LEU A | 10 | 13.304 | 4.825 | 39.331 | 1.00 | 31.86 | C |
| ATOM | 17 | N | ARG A | 11 | 14.000 | 0.143 | 38.166 | 1.00 | 32.98 | N |
| ATOM | 18 | CA | ARG A | 11 | 14.927 | -0.595 | 39.007 | 1.00 | 33.21 | C |
| ATOM | 19 | C | ARG A | 11 | 16.034 | 0.323 | 39.486 | 1.00 | 32.79 | C |
| ATOM | 20 | O | ARG A | 11 | 16.718 | 0.962 | 38.687 | 1.00 | 32.84 | O |
| ATOM | 21 | CB | ARG A | 11 | 15.513 | -1.791 | 38.259 | 1.00 | 33.61 | C |
| ATOM | 22 | CG | ARG A | 11 | 14.878 | -3.099 | 38.639 | 1.00 | 35.02 | C |
| ATOM | 23 | CD | ARG A | 11 | 14.193 | -3.810 | 37.493 | 1.00 | 37.55 | C |
| ATOM | 24 | NE | ARG A | 11 | 15.005 | -4.896 | 36.942 | 1.00 | 39.91 | N |
| ATOM | 25 | CZ | ARG A | 11 | 15.247 | -6.054 | 37.559 | 1.00 | 41.36 | C |
| ATOM | 26 | NH1 | ARG A | 11 | 15.994 | -6.977 | 36.964 | 1.00 | 42.17 | N |
| ATOM | 27 | NH2 | ARG A | 11 | 14.756 | -6.296 | 38.769 | 1.00 | 41.80 | N |
| ATOM | 28 | N | ILE A | 12 | 16.199 | 0.396 | 40.798 | 1.00 | 32.17 | N |
| ATOM | 29 | CA | ILE A | 12 | 17.286 | 1.170 | 41.367 | 1.00 | 31.92 | C |
| ATOM | 30 | C | ILE A | 12 | 18.427 | 0.204 | 41.656 | 1.00 | 31.86 | C |
| ATOM | 31 | O | ILE A | 12 | 18.321 | -0.656 | 42.531 | 1.00 | 31.99 | O |
| ATOM | 32 | CB | ILE A | 12 | 16.823 | 1.936 | 42.625 | 1.00 | 32.09 | C |
| ATOM | 33 | CG1 | ILE A | 12 | 15.554 | 2.741 | 42.311 | 1.00 | 30.95 | C |
| ATOM | 34 | CD1 | ILE A | 12 | 14.744 | 3.138 | 43.528 | 1.00 | 32.11 | C |
| ATOM | 35 | CG2 | ILE A | 12 | 17.961 | 2.838 | 43.161 | 1.00 | 31.67 | C |
| ATOM | 36 | N | LEU A | 13 | 19.508 | 0.345 | 40.894 | 1.00 | 31.41 | N |
| ATOM | 37 | CA | LEU A | 13 | 20.584 | -0.633 | 40.905 | 1.00 | 31.04 | C |
| ATOM | 38 | C | LEU A | 13 | 21.776 | -0.217 | 41.742 | 1.00 | 31.06 | C |
| ATOM | 39 | O | LEU A | 13 | 22.015 | 0.969 | 41.965 | 1.00 | 30.83 | O |
| ATOM | 40 | CB | LEU A | 13 | 21.037 | -0.968 | 39.476 | 1.00 | 31.01 | C |
| ATOM | 41 | CG | LEU A | 13 | 19.977 | -1.377 | 38.448 | 1.00 | 30.07 | C |
| ATOM | 42 | CD1 | LEU A | 13 | 20.614 | -1.480 | 37.085 | 1.00 | 29.65 | C |
| ATOM | 43 | CD2 | LEU A | 13 | 19.312 | -2.689 | 38.828 | 1.00 | 30.21 | C |
| ATOM | 44 | N | LYS A | 14 | 22.504 | -1.231 | 42.204 | 1.00 | 31.15 | N |
| ATOM | 45 | CA | LYS A | 14 | 23.772 | -1.084 | 42.906 | 1.00 | 31.49 | C |
| ATOM | 46 | C | LYS A | 14 | 24.890 | -1.119 | 41.873 | 1.00 | 31.65 | C |
| ATOM | 47 | O | LYS A | 14 | 24.764 | -1.801 | 40.849 | 1.00 | 31.42 | O |
| ATOM | 48 | CB | LYS A | 14 | 23.935 | -2.272 | 43.852 | 1.00 | 31.82 | C |
| ATOM | 49 | CG | LYS A | 14 | 24.780 | -2.033 | 45.069 | 1.00 | 32.02 | C |
| ATOM | 50 | CD | LYS A | 14 | 24.326 | -2.941 | 46.205 | 1.00 | 33.01 | C |
| ATOM | 51 | CE | LYS A | 14 | 24.637 | -4.406 | 45.932 | 1.00 | 32.29 | C |
| ATOM | 52 | NZ | LYS A | 14 | 24.743 | -5.168 | 47.198 | 1.00 | 33.27 | N |
| ATOM | 53 | N | GLU A | 15 | 25.989 | -0.418 | 42.146 | 1.00 | 31.81 | N |
| ATOM | 54 | CA | GLU A | 15 | 27.120 | -0.359 | 41.210 | 1.00 | 32.48 | C |

FIG. 5A

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 55 | C | GLU | A | 15 | 27.806 | -1.708 | 40.932 | 1.00 | 32.41 | C |
| ATOM | 56 | O | GLU | A | 15 | 28.520 | -1.843 | 39.930 | 1.00 | 32.25 | O |
| ATOM | 57 | CB | GLU | A | 15 | 28.146 | 0.697 | 41.647 | 1.00 | 32.94 | C |
| ATOM | 58 | CG | GLU | A | 15 | 29.148 | 0.224 | 42.692 | 1.00 | 34.55 | C |
| ATOM | 59 | CD | GLU | A | 15 | 29.762 | 1.362 | 43.481 | 1.00 | 36.00 | C |
| ATOM | 60 | OE1 | GLU | A | 15 | 29.775 | 2.496 | 42.967 | 1.00 | 37.36 | O |
| ATOM | 61 | OE2 | GLU | A | 15 | 30.241 | 1.124 | 44.616 | 1.00 | 36.70 | O |
| ATOM | 62 | N | THR | A | 16 | 27.579 | -2.695 | 41.803 | 1.00 | 32.34 | N |
| ATOM | 63 | CA | THR | A | 16 | 28.221 | -4.011 | 41.675 | 1.00 | 32.01 | C |
| ATOM | 64 | C | THR | A | 16 | 27.426 | -4.969 | 40.801 | 1.00 | 32.45 | C |
| ATOM | 65 | O | THR | A | 16 | 27.900 | -6.066 | 40.481 | 1.00 | 32.83 | O |
| ATOM | 66 | CB | THR | A | 16 | 28.429 | -4.668 | 43.052 | 1.00 | 32.11 | C |
| ATOM | 67 | OG1 | THR | A | 16 | 27.210 | -4.601 | 43.808 | 1.00 | 30.97 | O |
| ATOM | 68 | CG2 | THR | A | 16 | 29.442 | -3.896 | 43.879 | 1.00 | 31.66 | C |
| ATOM | 69 | N | GLU | A | 17 | 26.213 | -4.562 | 40.434 | 1.00 | 32.29 | N |
| ATOM | 70 | CA | GLU | A | 17 | 25.342 | -5.371 | 39.585 | 1.00 | 32.18 | C |
| ATOM | 71 | C | GLU | A | 17 | 25.581 | -5.121 | 38.091 | 1.00 | 31.51 | C |
| ATOM | 72 | O | GLU | A | 17 | 25.015 | -5.815 | 37.242 | 1.00 | 30.95 | O |
| ATOM | 73 | CB | GLU | A | 17 | 23.875 | -5.100 | 39.915 | 1.00 | 32.72 | C |
| ATOM | 74 | CG | GLU | A | 17 | 23.516 | -5.222 | 41.384 | 1.00 | 34.07 | C |
| ATOM | 75 | CD | GLU | A | 17 | 22.019 | -5.154 | 41.605 | 1.00 | 36.41 | C |
| ATOM | 76 | OE1 | GLU | A | 17 | 21.487 | -4.029 | 41.762 | 1.00 | 37.08 | O |
| ATOM | 77 | OE2 | GLU | A | 17 | 21.374 | -6.226 | 41.610 | 1.00 | 36.87 | O |
| ATOM | 78 | N | PHE | A | 18 | 26.402 | -4.121 | 37.774 | 1.00 | 30.88 | N |
| ATOM | 79 | CA | PHE | A | 18 | 26.700 | -3.792 | 36.382 | 1.00 | 30.61 | C |
| ATOM | 80 | C | PHE | A | 18 | 28.151 | -3.385 | 36.194 | 1.00 | 30.75 | C |
| ATOM | 81 | O | PHE | A | 18 | 28.791 | -2.904 | 37.121 | 1.00 | 31.58 | O |
| ATOM | 82 | CB | PHE | A | 18 | 25.725 | -2.733 | 35.816 | 1.00 | 29.96 | C |
| ATOM | 83 | CG | PHE | A | 18 | 25.812 | -1.390 | 36.493 | 1.00 | 28.54 | C |
| ATOM | 84 | CD1 | PHE | A | 18 | 26.686 | -0.412 | 36.022 | 1.00 | 27.16 | C |
| ATOM | 85 | CE1 | PHE | A | 18 | 26.775 | 0.832 | 36.646 | 1.00 | 27.02 | C |
| ATOM | 86 | CZ | PHE | A | 18 | 25.975 | 1.113 | 37.750 | 1.00 | 27.13 | C |
| ATOM | 87 | CE2 | PHE | A | 18 | 25.090 | 0.140 | 38.228 | 1.00 | 27.91 | C |
| ATOM | 88 | CD2 | PHE | A | 18 | 25.010 | -1.102 | 37.597 | 1.00 | 27.48 | C |
| ATOM | 89 | N | LYS | A | 19 | 28.665 | -3.584 | 34.988 | 1.00 | 31.19 | N |
| ATOM | 90 | CA | LYS | A | 19 | 30.030 | -3.194 | 34.661 | 1.00 | 31.21 | C |
| ATOM | 91 | C | LYS | A | 19 | 30.057 | -2.449 | 33.335 | 1.00 | 31.16 | C |
| ATOM | 92 | O | LYS | A | 19 | 29.541 | -2.943 | 32.330 | 1.00 | 30.67 | O |
| ATOM | 93 | CB | LYS | A | 19 | 30.930 | -4.430 | 34.576 | 1.00 | 31.45 | C |
| ATOM | 94 | CG | LYS | A | 19 | 31.761 | -4.681 | 35.822 | 1.00 | 32.26 | C |
| ATOM | 95 | N | LYS | A | 20 | 30.654 | -1.260 | 33.341 | 1.00 | 31.15 | N |
| ATOM | 96 | CA | LYS | A | 20 | 30.934 | -0.546 | 32.105 | 1.00 | 31.40 | C |
| ATOM | 97 | C | LYS | A | 20 | 32.021 | -1.321 | 31.374 | 1.00 | 31.40 | C |
| ATOM | 98 | O | LYS | A | 20 | 33.053 | -1.639 | 31.956 | 1.00 | 31.52 | O |
| ATOM | 99 | CB | LYS | A | 20 | 31.399 | 0.889 | 32.376 | 1.00 | 31.51 | C |
| ATOM | 100 | CG | LYS | A | 20 | 30.380 | 1.782 | 33.069 | 1.00 | 31.94 | C |
| ATOM | 101 | CD | LYS | A | 20 | 30.794 | 3.245 | 33.003 | 1.00 | 33.29 | C |
| ATOM | 102 | CE | LYS | A | 20 | 31.526 | 3.728 | 34.258 | 1.00 | 33.37 | C |
| ATOM | 103 | NZ | LYS | A | 20 | 30.997 | 3.136 | 35.524 | 1.00 | 34.90 | N |
| ATOM | 104 | N | ILE | A | 21 | 31.783 | -1.635 | 30.105 | 1.00 | 31.30 | N |
| ATOM | 105 | CA | ILE | A | 21 | 32.736 | -2.418 | 29.325 | 1.00 | 31.02 | C |
| ATOM | 106 | C | ILE | A | 21 | 33.404 | -1.615 | 28.202 | 1.00 | 30.87 | C |
| ATOM | 107 | O | ILE | A | 21 | 34.594 | -1.777 | 27.950 | 1.00 | 31.27 | O |
| ATOM | 108 | CB | ILE | A | 21 | 32.067 | -3.740 | 28.829 | 1.00 | 31.23 | C |
| ATOM | 109 | CG1 | ILE | A | 21 | 32.623 | -4.940 | 29.605 | 1.00 | 30.99 | C |
| ATOM | 110 | CD1 | ILE | A | 21 | 31.921 | -5.212 | 30.914 | 1.00 | 30.77 | C |
| ATOM | 111 | CG2 | ILE | A | 21 | 32.234 | -3.966 | 27.325 | 1.00 | 31.85 | C |
| ATOM | 112 | N | LYS | A | 22 | 32.652 | -0.737 | 27.544 | 1.00 | 30.35 | N |
| ATOM | 113 | CA | LYS | A | 22 | 33.167 | -0.045 | 26.368 | 1.00 | 29.67 | C |
| ATOM | 114 | C | LYS | A | 22 | 32.485 | 1.303 | 26.166 | 1.00 | 28.92 | C |

FIG. 5B

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 115 | O | LYS | A | 22 | 31.291 | 1.447 | 26.430 | 1.00 | 28.97 | O |
| ATOM | 116 | CB | LYS | A | 22 | 32.994 | -0.944 | 25.131 | 1.00 | 29.91 | C |
| ATOM | 117 | CG | LYS | A | 22 | 33.463 | -0.353 | 23.807 | 1.00 | 31.31 | C |
| ATOM | 118 | CD | LYS | A | 22 | 32.584 | -0.846 | 22.663 | 1.00 | 33.69 | C |
| ATOM | 119 | CE | LYS | A | 22 | 32.824 | -0.061 | 21.384 | 1.00 | 34.84 | C |
| ATOM | 120 | NZ | LYS | A | 22 | 33.873 | -0.701 | 20.548 | 1.00 | 35.55 | N |
| ATOM | 121 | N | VAL | A | 23 | 33.247 | 2.291 | 25.702 | 1.00 | 27.85 | N |
| ATOM | 122 | CA | VAL | A | 23 | 32.673 | 3.572 | 25.319 | 1.00 | 26.80 | C |
| ATOM | 123 | C | VAL | A | 23 | 31.989 | 3.441 | 23.955 | 1.00 | 26.47 | C |
| ATOM | 124 | O | VAL | A | 23 | 32.578 | 2.927 | 23.007 | 1.00 | 26.06 | O |
| ATOM | 125 | CB | VAL | A | 23 | 33.731 | 4.714 | 25.304 | 1.00 | 27.14 | C |
| ATOM | 126 | CG1 | VAL | A | 23 | 33.159 | 5.975 | 24.668 | 1.00 | 25.33 | C |
| ATOM | 127 | CG2 | VAL | A | 23 | 34.220 | 5.013 | 26.709 | 1.00 | 25.82 | C |
| ATOM | 128 | N | LEU | A | 24 | 30.736 | 3.889 | 23.882 | 1.00 | 26.11 | N |
| ATOM | 129 | CA | LEU | A | 24 | 29.947 | 3.842 | 22.655 | 1.00 | 25.98 | C |
| ATOM | 130 | C | LEU | A | 24 | 29.745 | 5.224 | 22.047 | 1.00 | 26.08 | C |
| ATOM | 131 | O | LEU | A | 24 | 29.515 | 5.356 | 20.841 | 1.00 | 26.32 | O |
| ATOM | 132 | CB | LEU | A | 24 | 28.572 | 3.243 | 22.929 | 1.00 | 26.10 | C |
| ATOM | 133 | CG | LEU | A | 24 | 28.399 | 1.794 | 23.364 | 1.00 | 26.00 | C |
| ATOM | 134 | CD1 | LEU | A | 24 | 26.914 | 1.572 | 23.585 | 1.00 | 25.49 | C |
| ATOM | 135 | CD2 | LEU | A | 24 | 28.954 | 0.810 | 22.341 | 1.00 | 25.35 | C |
| ATOM | 136 | N | GLY | A | 25 | 29.809 | 6.249 | 22.888 | 1.00 | 25.98 | N |
| ATOM | 137 | CA | GLY | A | 25 | 29.611 | 7.607 | 22.440 | 1.00 | 26.07 | C |
| ATOM | 138 | C | GLY | A | 25 | 29.361 | 8.580 | 23.571 | 1.00 | 26.33 | C |
| ATOM | 139 | O | GLY | A | 25 | 29.640 | 8.284 | 24.732 | 1.00 | 26.03 | O |
| ATOM | 140 | N | SER | A | 26 | 28.829 | 9.746 | 23.214 | 1.00 | 26.48 | N |
| ATOM | 141 | CA | SER | A | 26 | 28.651 | 10.849 | 24.150 | 1.00 | 27.44 | C |
| ATOM | 142 | C | SER | A | 26 | 27.703 | 11.912 | 23.601 | 1.00 | 27.82 | C |
| ATOM | 143 | O | SER | A | 26 | 27.468 | 11.996 | 22.393 | 1.00 | 27.97 | O |
| ATOM | 144 | CB | SER | A | 26 | 30.002 | 11.488 | 24.477 | 1.00 | 27.22 | C |
| ATOM | 145 | OG | SER | A | 26 | 30.508 | 12.178 | 23.346 | 1.00 | 28.14 | O |
| ATOM | 146 | N | GLY | A | 27 | 27.160 | 12.721 | 24.505 | 1.00 | 28.49 | N |
| ATOM | 147 | CA | GLY | A | 27 | 26.332 | 13.845 | 24.129 | 1.00 | 28.72 | C |
| ATOM | 148 | C | GLY | A | 27 | 26.493 | 14.972 | 25.122 | 1.00 | 29.64 | C |
| ATOM | 149 | O | GLY | A | 27 | 27.458 | 15.007 | 25.902 | 1.00 | 29.14 | O |
| ATOM | 150 | N | ALA | A | 28 | 25.531 | 15.893 | 25.091 | 1.00 | 30.01 | N |
| ATOM | 151 | CA | ALA | A | 28 | 25.513 | 17.052 | 25.970 | 1.00 | 30.43 | C |
| ATOM | 152 | C | ALA | A | 28 | 25.262 | 16.704 | 27.442 | 1.00 | 30.90 | C |
| ATOM | 153 | O | ALA | A | 28 | 25.416 | 17.561 | 28.307 | 1.00 | 31.78 | O |
| ATOM | 154 | CB | ALA | A | 28 | 24.475 | 18.063 | 25.477 | 1.00 | 30.69 | C |
| ATOM | 155 | N | PHE | A | 29 | 24.888 | 15.458 | 27.729 | 1.00 | 30.85 | N |
| ATOM | 156 | CA | PHE | A | 29 | 24.550 | 15.066 | 29.097 | 1.00 | 31.31 | C |
| ATOM | 157 | C | PHE | A | 29 | 25.490 | 14.028 | 29.714 | 1.00 | 30.84 | C |
| ATOM | 158 | O | PHE | A | 29 | 25.353 | 13.681 | 30.887 | 1.00 | 30.79 | O |
| ATOM | 159 | CB | PHE | A | 29 | 23.087 | 14.616 | 29.184 | 1.00 | 31.85 | C |
| ATOM | 160 | CG | PHE | A | 29 | 22.111 | 15.610 | 28.605 | 1.00 | 33.49 | C |
| ATOM | 161 | CD1 | PHE | A | 29 | 22.080 | 16.928 | 29.063 | 1.00 | 34.55 | C |
| ATOM | 162 | CE1 | PHE | A | 29 | 21.182 | 17.851 | 28.532 | 1.00 | 34.83 | C |
| ATOM | 163 | CZ | PHE | A | 29 | 20.307 | 17.462 | 27.528 | 1.00 | 34.78 | C |
| ATOM | 164 | CE2 | PHE | A | 29 | 20.325 | 16.147 | 27.062 | 1.00 | 35.55 | C |
| ATOM | 165 | CD2 | PHE | A | 29 | 21.230 | 15.231 | 27.598 | 1.00 | 34.07 | C |
| ATOM | 166 | N | GLY | A | 30 | 26.444 | 13.540 | 28.930 | 1.00 | 30.40 | N |
| ATOM | 167 | CA | GLY | A | 30 | 27.493 | 12.693 | 29.468 | 1.00 | 29.90 | C |
| ATOM | 168 | C | GLY | A | 30 | 28.079 | 11.704 | 28.483 | 1.00 | 29.36 | C |
| ATOM | 169 | O | GLY | A | 30 | 28.136 | 11.957 | 27.278 | 1.00 | 29.36 | O |
| ATOM | 170 | N | THR | A | 31 | 28.511 | 10.566 | 29.011 | 1.00 | 28.32 | N |
| ATOM | 171 | CA | THR | A | 31 | 29.150 | 9.534 | 28.213 | 1.00 | 27.45 | C |
| ATOM | 172 | C | THR | A | 31 | 28.284 | 8.286 | 28.200 | 1.00 | 27.34 | C |
| ATOM | 173 | O | THR | A | 31 | 27.704 | 7.911 | 29.231 | 1.00 | 27.24 | O |
| ATOM | 174 | CB | THR | A | 31 | 30.542 | 9.214 | 28.788 | 1.00 | 27.08 | C |

FIG. 5C

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 175 | OG1 | THR | A | 31 | 31.321 | 10.418 | 28.841 | 1.00 | 26.63 | O |
| ATOM | 176 | CG2 | THR | A | 31 | 31.329 | 8.308 | 27.848 | 1.00 | 25.44 | C |
| ATOM | 177 | N | VAL | A | 32 | 28.206 | 7.651 | 27.034 | 1.00 | 26.41 | N |
| ATOM | 178 | CA | VAL | A | 32 | 27.445 | 6.419 | 26.881 | 1.00 | 26.25 | C |
| ATOM | 179 | C | VAL | A | 32 | 28.392 | 5.219 | 26.785 | 1.00 | 26.12 | C |
| ATOM | 180 | O | VAL | A | 32 | 29.306 | 5.188 | 25.954 | 1.00 | 25.73 | O |
| ATOM | 181 | CB | VAL | A | 32 | 26.480 | 6.464 | 25.652 | 1.00 | 26.51 | C |
| ATOM | 182 | CG1 | VAL | A | 32 | 25.591 | 5.231 | 25.621 | 1.00 | 26.16 | C |
| ATOM | 183 | CG2 | VAL | A | 32 | 25.621 | 7.738 | 25.659 | 1.00 | 26.08 | C |
| ATOM | 184 | N | TYR | A | 33 | 28.152 | 4.234 | 27.644 | 1.00 | 25.90 | N |
| ATOM | 185 | CA | TYR | A | 33 | 28.914 | 2.993 | 27.643 | 1.00 | 25.79 | C |
| ATOM | 186 | C | TYR | A | 33 | 28.051 | 1.802 | 27.277 | 1.00 | 25.73 | C |
| ATOM | 187 | O | TYR | A | 33 | 26.841 | 1.804 | 27.488 | 1.00 | 25.45 | O |
| ATOM | 188 | CB | TYR | A | 33 | 29.505 | 2.729 | 29.024 | 1.00 | 25.52 | C |
| ATOM | 189 | CG | TYR | A | 33 | 30.458 | 3.780 | 29.518 | 1.00 | 25.63 | C |
| ATOM | 190 | CD1 | TYR | A | 33 | 29.991 | 4.976 | 30.056 | 1.00 | 26.29 | C |
| ATOM | 191 | CE1 | TYR | A | 33 | 30.872 | 5.943 | 30.525 | 1.00 | 26.43 | C |
| ATOM | 192 | CZ | TYR | A | 33 | 32.230 | 5.703 | 30.455 | 1.00 | 26.84 | C |
| ATOM | 193 | OH | TYR | A | 33 | 33.113 | 6.644 | 30.912 | 1.00 | 28.91 | O |
| ATOM | 194 | CE2 | TYR | A | 33 | 32.714 | 4.524 | 29.931 | 1.00 | 26.56 | C |
| ATOM | 195 | CD2 | TYR | A | 33 | 31.833 | 3.570 | 29.470 | 1.00 | 26.17 | C |
| ATOM | 196 | N | LYS | A | 34 | 28.690 | 0.780 | 26.724 | 1.00 | 26.11 | N |
| ATOM | 197 | CA | LYS | A | 34 | 28.119 | -0.553 | 26.713 | 1.00 | 26.19 | C |
| ATOM | 198 | C | LYS | A | 34 | 28.528 | -1.189 | 28.034 | 1.00 | 26.36 | C |
| ATOM | 199 | O | LYS | A | 34 | 29.629 | -0.947 | 28.539 | 1.00 | 26.37 | O |
| ATOM | 200 | CB | LYS | A | 34 | 28.647 | -1.374 | 25.536 | 1.00 | 26.34 | C |
| ATOM | 201 | CG | LYS | A | 34 | 28.254 | -2.854 | 25.578 | 1.00 | 26.67 | C |
| ATOM | 202 | CD | LYS | A | 34 | 28.699 | -3.591 | 24.324 | 1.00 | 28.28 | C |
| ATOM | 203 | CE | LYS | A | 34 | 30.209 | -3.644 | 24.207 | 1.00 | 28.80 | C |
| ATOM | 204 | NZ | LYS | A | 34 | 30.651 | -4.626 | 23.185 | 1.00 | 29.64 | N |
| ATOM | 205 | N | GLY | A | 35 | 27.633 | -1.982 | 28.601 | 1.00 | 26.48 | N |
| ATOM | 206 | CA | GLY | A | 35 | 27.916 | -2.655 | 29.846 | 1.00 | 27.05 | C |
| ATOM | 207 | C | GLY | A | 35 | 27.283 | -4.021 | 29.931 | 1.00 | 27.50 | C |
| ATOM | 208 | O | GLY | A | 35 | 26.579 | -4.461 | 29.016 | 1.00 | 27.33 | O |
| ATOM | 209 | N | LEU | A | 36 | 27.569 | -4.704 | 31.031 | 1.00 | 28.07 | N |
| ATOM | 210 | CA | LEU | A | 36 | 26.910 | -5.965 | 31.346 | 1.00 | 28.83 | C |
| ATOM | 211 | C | LEU | A | 36 | 26.159 | -5.815 | 32.651 | 1.00 | 29.31 | C |
| ATOM | 212 | O | LEU | A | 36 | 26.651 | -5.203 | 33.608 | 1.00 | 28.70 | O |
| ATOM | 213 | CB | LEU | A | 36 | 27.907 | -7.122 | 31.413 | 1.00 | 28.61 | C |
| ATOM | 214 | CG | LEU | A | 36 | 28.522 | -7.486 | 30.057 | 1.00 | 29.10 | C |
| ATOM | 215 | CD1 | LEU | A | 36 | 29.704 | -8.429 | 30.235 | 1.00 | 29.07 | C |
| ATOM | 216 | CD2 | LEU | A | 36 | 27.481 | -8.074 | 29.099 | 1.00 | 27.73 | C |
| ATOM | 217 | N | TRP | A | 37 | 24.953 | -6.366 | 32.662 | 1.00 | 30.29 | N |
| ATOM | 218 | CA | TRP | A | 37 | 24.050 | -6.257 | 33.794 | 1.00 | 31.66 | C |
| ATOM | 219 | C | TRP | A | 37 | 23.555 | -7.649 | 34.178 | 1.00 | 32.41 | C |
| ATOM | 220 | O | TRP | A | 37 | 23.057 | -8.398 | 33.337 | 1.00 | 32.28 | O |
| ATOM | 221 | CB | TRP | A | 37 | 22.885 | -5.325 | 33.431 | 1.00 | 31.36 | C |
| ATOM | 222 | CG | TRP | A | 37 | 21.749 | -5.309 | 34.400 | 1.00 | 31.84 | C |
| ATOM | 223 | CD1 | TRP | A | 37 | 21.827 | -5.288 | 35.765 | 1.00 | 31.66 | C |
| ATOM | 224 | NE1 | TRP | A | 37 | 20.568 | -5.278 | 36.312 | 1.00 | 31.87 | N |
| ATOM | 225 | CE2 | TRP | A | 37 | 19.643 | -5.284 | 35.303 | 1.00 | 32.18 | C |
| ATOM | 226 | CD2 | TRP | A | 37 | 20.355 | -5.302 | 34.080 | 1.00 | 32.48 | C |
| ATOM | 227 | CE3 | TRP | A | 37 | 19.627 | -5.315 | 32.881 | 1.00 | 32.93 | C |
| ATOM | 228 | CZ3 | TRP | A | 37 | 18.234 | -5.305 | 32.939 | 1.00 | 34.29 | C |
| ATOM | 229 | CH2 | TRP | A | 37 | 17.558 | -5.288 | 34.173 | 1.00 | 34.07 | C |
| ATOM | 230 | CZ2 | TRP | A | 37 | 18.246 | -5.275 | 35.363 | 1.00 | 33.37 | C |
| ATOM | 231 | N | ILE | A | 38 | 23.728 | -7.998 | 35.446 | 1.00 | 33.59 | N |
| ATOM | 232 | CA | ILE | A | 38 | 23.151 | -9.220 | 35.986 | 1.00 | 35.00 | C |
| ATOM | 233 | C | ILE | A | 38 | 21.966 | -8.808 | 36.844 | 1.00 | 36.18 | C |
| ATOM | 234 | O | ILE | A | 38 | 22.149 | -8.219 | 37.915 | 1.00 | 36.19 | O |

FIG. 5D

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|---------|--------|------|-------|---|
| ATOM | 235 | CB | ILE | A | 38 | 24.198 | -10.037 | 36.802 | 1.00 | 35.17 | C |
| ATOM | 236 | CG1 | ILE | A | 38 | 25.308 | -10.562 | 35.888 | 1.00 | 34.19 | C |
| ATOM | 237 | CD1 | ILE | A | 38 | 26.688 | -10.346 | 36.435 | 1.00 | 33.99 | C |
| ATOM | 238 | CG2 | ILE | A | 38 | 23.532 | -11.213 | 37.543 | 1.00 | 35.42 | C |
| ATOM | 239 | N | PRO | A | 39 | 20.755 | -9.090 | 36.362 | 1.00 | 37.54 | N |
| ATOM | 240 | CA | PRO | A | 39 | 19.532 | -8.772 | 37.106 | 1.00 | 38.74 | C |
| ATOM | 241 | C | PRO | A | 39 | 19.432 | -9.599 | 38.383 | 1.00 | 39.96 | C |
| ATOM | 242 | O | PRO | A | 39 | 20.073 | -10.652 | 38.495 | 1.00 | 40.58 | O |
| ATOM | 243 | CB | PRO | A | 39 | 18.417 | -9.156 | 36.130 | 1.00 | 38.70 | C |
| ATOM | 244 | CG | PRO | A | 39 | 19.070 | -9.245 | 34.812 | 1.00 | 38.09 | C |
| ATOM | 245 | CD | PRO | A | 39 | 20.455 | -9.737 | 35.073 | 1.00 | 37.80 | C |
| ATOM | 246 | N | GLU | A | 40 | 18.643 | -9.114 | 39.335 | 1.00 | 41.45 | N |
| ATOM | 247 | CA | GLU | A | 40 | 18.572 | -9.711 | 40.665 | 1.00 | 42.64 | C |
| ATOM | 248 | C | GLU | A | 40 | 17.938 | -11.104 | 40.655 | 1.00 | 43.47 | C |
| ATOM | 249 | O | GLU | A | 40 | 16.830 | -11.301 | 40.153 | 1.00 | 43.34 | O |
| ATOM | 250 | CB | GLU | A | 40 | 17.836 | -8.777 | 41.630 | 1.00 | 42.63 | C |
| ATOM | 251 | N | GLY | A | 41 | 18.668 | -12.065 | 41.211 | 1.00 | 44.81 | N |
| ATOM | 252 | CA | GLY | A | 41 | 18.222 | -13.444 | 41.277 | 1.00 | 45.93 | C |
| ATOM | 253 | C | GLY | A | 41 | 18.849 | -14.292 | 40.188 | 1.00 | 46.56 | C |
| ATOM | 254 | O | GLY | A | 41 | 19.423 | -15.345 | 40.465 | 1.00 | 46.81 | O |
| ATOM | 255 | N | GLU | A | 42 | 18.742 | -13.817 | 38.949 | 1.00 | 47.24 | N |
| ATOM | 256 | CA | GLU | A | 42 | 19.230 | -14.539 | 37.776 | 1.00 | 47.50 | C |
| ATOM | 257 | C | GLU | A | 42 | 20.757 | -14.586 | 37.728 | 1.00 | 47.53 | C |
| ATOM | 258 | O | GLU | A | 42 | 21.433 | -13.986 | 38.567 | 1.00 | 48.02 | O |
| ATOM | 259 | CB | GLU | A | 42 | 18.664 | -13.930 | 36.489 | 1.00 | 47.70 | C |
| ATOM | 260 | CG | GLU | A | 42 | 17.949 | -12.598 | 36.672 | 1.00 | 48.46 | C |
| ATOM | 261 | CD | GLU | A | 42 | 16.805 | -12.393 | 35.693 | 1.00 | 49.13 | C |
| ATOM | 262 | OE1 | GLU | A | 42 | 15.745 | -11.880 | 36.117 | 1.00 | 49.77 | O |
| ATOM | 263 | OE2 | GLU | A | 42 | 16.960 | -12.732 | 34.500 | 1.00 | 49.24 | O |
| ATOM | 264 | N | LYS | A | 43 | 21.293 | -15.314 | 36.753 | 1.00 | 47.44 | N |
| ATOM | 265 | CA | LYS | A | 43 | 22.737 | -15.466 | 36.612 | 1.00 | 46.89 | C |
| ATOM | 266 | C | LYS | A | 43 | 23.248 | -14.807 | 35.336 | 1.00 | 46.48 | C |
| ATOM | 267 | O | LYS | A | 43 | 24.414 | -14.406 | 35.262 | 1.00 | 46.92 | O |
| ATOM | 268 | CB | LYS | A | 43 | 23.122 | -16.946 | 36.638 | 1.00 | 47.10 | C |
| ATOM | 269 | N | VAL | A | 44 | 22.368 | -14.685 | 34.346 | 1.00 | 45.53 | N |
| ATOM | 270 | CA | VAL | A | 44 | 22.731 | -14.147 | 33.037 | 1.00 | 44.72 | C |
| ATOM | 271 | C | VAL | A | 44 | 23.259 | -12.716 | 33.085 | 1.00 | 43.92 | C |
| ATOM | 272 | O | VAL | A | 44 | 22.697 | -11.853 | 33.775 | 1.00 | 44.20 | O |
| ATOM | 273 | CB | VAL | A | 44 | 21.554 | -14.197 | 32.029 | 1.00 | 44.84 | C |
| ATOM | 274 | CG1 | VAL | A | 44 | 22.026 | -14.763 | 30.704 | 1.00 | 44.64 | C |
| ATOM | 275 | CG2 | VAL | A | 44 | 20.376 | -15.005 | 32.581 | 1.00 | 45.38 | C |
| ATOM | 276 | N | LYS | A | 45 | 24.346 | -12.484 | 32.350 | 1.00 | 42.20 | N |
| ATOM | 277 | CA | LYS | A | 45 | 24.859 | -11.144 | 32.113 | 1.00 | 40.90 | C |
| ATOM | 278 | C | LYS | A | 45 | 24.220 | -10.570 | 30.847 | 1.00 | 39.86 | C |
| ATOM | 279 | O | LYS | A | 45 | 24.362 | -11.136 | 29.758 | 1.00 | 39.98 | O |
| ATOM | 280 | CB | LYS | A | 45 | 26.384 | -11.163 | 31.997 | 1.00 | 40.99 | C |
| ATOM | 281 | N | ILE | A | 46 | 23.514 | -9.450 | 31.007 | 1.00 | 38.25 | N |
| ATOM | 282 | CA | ILE | A | 46 | 22.746 | -8.819 | 29.928 | 1.00 | 36.38 | C |
| ATOM | 283 | C | ILE | A | 46 | 23.442 | -7.555 | 29.394 | 1.00 | 34.87 | C |
| ATOM | 284 | O | ILE | A | 46 | 23.656 | -6.607 | 30.151 | 1.00 | 35.08 | O |
| ATOM | 285 | CB | ILE | A | 46 | 21.309 | -8.474 | 30.421 | 1.00 | 36.31 | C |
| ATOM | 286 | CG1 | ILE | A | 46 | 20.488 | -9.751 | 30.621 | 1.00 | 36.62 | C |
| ATOM | 287 | CD1 | ILE | A | 46 | 19.140 | -9.537 | 31.301 | 1.00 | 36.72 | C |
| ATOM | 288 | CG2 | ILE | A | 46 | 20.603 | -7.520 | 29.446 | 1.00 | 36.09 | C |
| ATOM | 289 | N | PRO | A | 47 | 23.794 | -7.542 | 28.104 | 1.00 | 33.01 | N |
| ATOM | 290 | CA | PRO | A | 47 | 24.351 | -6.338 | 27.475 | 1.00 | 31.20 | C |
| ATOM | 291 | C | PRO | A | 47 | 23.350 | -5.179 | 27.476 | 1.00 | 29.44 | C |
| ATOM | 292 | O | PRO | A | 47 | 22.178 | -5.343 | 27.103 | 1.00 | 29.35 | O |
| ATOM | 293 | CB | PRO | A | 47 | 24.688 | -6.793 | 26.046 | 1.00 | 31.38 | C |
| ATOM | 294 | CG | PRO | A | 47 | 23.887 | -8.026 | 25.818 | 1.00 | 32.45 | C |

FIG. 5E

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 295 | CD | PRO | A | 47 | 23.714 | -8.674 | 27.161 | 1.00 | 33.23 | C |
| ATOM | 296 | N | VAL | A | 48 | 23.823 | -4.020 | 27.922 | 1.00 | 26.93 | N |
| ATOM | 297 | CA | VAL | A | 48 | 22.989 | -2.832 | 28.098 | 1.00 | 24.82 | C |
| ATOM | 298 | C | VAL | A | 48 | 23.769 | -1.576 | 27.731 | 1.00 | 24.03 | C |
| ATOM | 299 | O | VAL | A | 48 | 24.996 | -1.607 | 27.605 | 1.00 | 22.88 | O |
| ATOM | 300 | CB | VAL | A | 48 | 22.509 | -2.666 | 29.577 | 1.00 | 24.76 | C |
| ATOM | 301 | CG1 | VAL | A | 48 | 21.516 | -3.761 | 29.985 | 1.00 | 23.63 | C |
| ATOM | 302 | CG2 | VAL | A | 48 | 23.700 | -2.600 | 30.544 | 1.00 | 23.66 | C |
| ATOM | 303 | N | ALA | A | 49 | 23.049 | -0.471 | 27.578 | 1.00 | 22.99 | N |
| ATOM | 304 | CA | ALA | A | 49 | 23.679 | 0.835 | 27.509 | 1.00 | 22.69 | C |
| ATOM | 305 | C | ALA | A | 49 | 23.653 | 1.498 | 28.883 | 1.00 | 22.56 | C |
| ATOM | 306 | O | ALA | A | 49 | 22.621 | 1.525 | 29.558 | 1.00 | 22.34 | O |
| ATOM | 307 | CB | ALA | A | 49 | 22.994 | 1.720 | 26.456 | 1.00 | 22.34 | C |
| ATOM | 308 | N | ILE | A | 50 | 24.804 | 2.019 | 29.290 | 1.00 | 23.08 | N |
| ATOM | 309 | CA | ILE | A | 50 | 24.934 | 2.780 | 30.530 | 1.00 | 23.05 | C |
| ATOM | 310 | C | ILE | A | 50 | 25.331 | 4.225 | 30.254 | 1.00 | 22.95 | C |
| ATOM | 311 | O | ILE | A | 50 | 26.410 | 4.497 | 29.737 | 1.00 | 22.99 | O |
| ATOM | 312 | CB | ILE | A | 50 | 25.944 | 2.122 | 31.499 | 1.00 | 22.68 | C |
| ATOM | 313 | CG1 | ILE | A | 50 | 25.600 | 0.646 | 31.724 | 1.00 | 23.20 | C |
| ATOM | 314 | CD1 | ILE | A | 50 | 26.767 | -0.183 | 32.250 | 1.00 | 23.10 | C |
| ATOM | 315 | CG2 | ILE | A | 50 | 25.983 | 2.883 | 32.828 | 1.00 | 22.78 | C |
| ATOM | 316 | N | LYS | A | 51 | 24.452 | 5.144 | 30.614 | 1.00 | 23.57 | N |
| ATOM | 317 | CA | LYS | A | 51 | 24.721 | 6.564 | 30.464 | 1.00 | 25.45 | C |
| ATOM | 318 | C | LYS | A | 51 | 25.241 | 7.140 | 31.790 | 1.00 | 26.16 | C |
| ATOM | 319 | O | LYS | A | 51 | 24.565 | 7.081 | 32.809 | 1.00 | 26.54 | O |
| ATOM | 320 | CB | LYS | A | 51 | 23.457 | 7.288 | 29.998 | 1.00 | 25.27 | C |
| ATOM | 321 | CG | LYS | A | 51 | 23.718 | 8.519 | 29.142 | 1.00 | 27.21 | C |
| ATOM | 322 | N | GLU | A | 52 | 26.462 | 7.659 | 31.769 | 1.00 | 27.10 | N |
| ATOM | 323 | CA | GLU | A | 52 | 27.046 | 8.307 | 32.932 | 1.00 | 28.25 | C |
| ATOM | 324 | C | GLU | A | 52 | 26.848 | 9.812 | 32.796 | 1.00 | 28.35 | C |
| ATOM | 325 | O | GLU | A | 52 | 27.412 | 10.439 | 31.900 | 1.00 | 28.29 | O |
| ATOM | 326 | CB | GLU | A | 52 | 28.538 | 7.966 | 33.051 | 1.00 | 28.46 | C |
| ATOM | 327 | CG | GLU | A | 52 | 28.883 | 7.152 | 34.284 | 1.00 | 30.20 | C |
| ATOM | 328 | CD | GLU | A | 52 | 30.303 | 7.358 | 34.796 | 1.00 | 31.24 | C |
| ATOM | 329 | OE1 | GLU | A | 52 | 31.218 | 7.648 | 33.998 | 1.00 | 32.93 | O |
| ATOM | 330 | OE2 | GLU | A | 52 | 30.513 | 7.203 | 36.012 | 1.00 | 31.33 | O |
| ATOM | 331 | N | LEU | A | 53 | 26.034 | 10.387 | 33.675 | 1.00 | 29.03 | N |
| ATOM | 332 | CA | LEU | A | 53 | 25.664 | 11.796 | 33.553 | 1.00 | 29.57 | C |
| ATOM | 333 | C | LEU | A | 53 | 26.732 | 12.715 | 34.106 | 1.00 | 30.34 | C |
| ATOM | 334 | O | LEU | A | 53 | 27.415 | 12.382 | 35.076 | 1.00 | 31.05 | O |
| ATOM | 335 | CB | LEU | A | 53 | 24.328 | 12.083 | 34.245 | 1.00 | 29.20 | C |
| ATOM | 336 | CG | LEU | A | 53 | 23.069 | 11.285 | 33.895 | 1.00 | 28.26 | C |
| ATOM | 337 | CD1 | LEU | A | 53 | 21.861 | 11.971 | 34.515 | 1.00 | 26.83 | C |
| ATOM | 338 | CD2 | LEU | A | 53 | 22.879 | 11.103 | 32.389 | 1.00 | 28.29 | C |
| ATOM | 339 | N | ARG | A | 54 | 26.870 | 13.875 | 33.474 | 1.00 | 31.28 | N |
| ATOM | 340 | CA | ARG | A | 54 | 27.786 | 14.916 | 33.928 | 1.00 | 31.73 | C |
| ATOM | 341 | C | ARG | A | 54 | 27.358 | 15.412 | 35.308 | 1.00 | 32.02 | C |
| ATOM | 342 | O | ARG | A | 54 | 26.163 | 15.592 | 35.562 | 1.00 | 32.31 | O |
| ATOM | 343 | CB | ARG | A | 54 | 27.789 | 16.080 | 32.931 | 1.00 | 31.78 | C |
| ATOM | 344 | N | SER | A | 58 | 19.539 | 24.051 | 39.068 | 1.00 | 50.63 | N |
| ATOM | 345 | CA | SER | A | 58 | 20.284 | 23.063 | 38.287 | 1.00 | 50.22 | C |
| ATOM | 346 | C | SER | A | 58 | 20.680 | 21.820 | 39.109 | 1.00 | 49.81 | C |
| ATOM | 347 | O | SER | A | 58 | 20.399 | 20.698 | 38.676 | 1.00 | 50.12 | O |
| ATOM | 348 | CB | SER | A | 58 | 21.494 | 23.706 | 37.597 | 1.00 | 50.55 | C |
| ATOM | 349 | OG | SER | A | 58 | 21.122 | 24.917 | 36.951 | 1.00 | 51.16 | O |
| ATOM | 350 | N | PRO | A | 59 | 21.322 | 21.991 | 40.270 | 1.00 | 48.85 | N |
| ATOM | 351 | CA | PRO | A | 59 | 21.537 | 20.860 | 41.182 | 1.00 | 48.01 | C |
| ATOM | 352 | C | PRO | A | 59 | 20.206 | 20.364 | 41.754 | 1.00 | 46.81 | C |
| ATOM | 353 | O | PRO | A | 59 | 19.345 | 21.180 | 42.112 | 1.00 | 46.82 | O |
| ATOM | 354 | CB | PRO | A | 59 | 22.412 | 21.459 | 42.287 | 1.00 | 48.31 | C |

FIG. 5F

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 355 | CG | PRO | A | 59 | 23.010 | 22.670 | 41.671 | 1.00 | 48.96 | C |
| ATOM | 356 | CD | PRO | A | 59 | 21.917 | 23.228 | 40.807 | 1.00 | 49.26 | C |
| ATOM | 357 | N | LYS | A | 60 | 20.048 | 19.044 | 41.827 | 1.00 | 44.81 | N |
| ATOM | 358 | CA | LYS | A | 60 | 18.764 | 18.438 | 42.154 | 1.00 | 43.01 | C |
| ATOM | 359 | C | LYS | A | 60 | 18.870 | 17.419 | 43.282 | 1.00 | 41.79 | C |
| ATOM | 360 | O | LYS | A | 60 | 19.883 | 16.735 | 43.424 | 1.00 | 41.70 | O |
| ATOM | 361 | CB | LYS | A | 60 | 18.167 | 17.775 | 40.910 | 1.00 | 43.20 | C |
| ATOM | 362 | N | ALA | A | 61 | 17.813 | 17.327 | 44.081 | 1.00 | 40.01 | N |
| ATOM | 363 | CA | ALA | A | 61 | 17.735 | 16.332 | 45.136 | 1.00 | 38.28 | C |
| ATOM | 364 | C | ALA | A | 61 | 17.434 | 14.973 | 44.528 | 1.00 | 37.38 | C |
| ATOM | 365 | O | ALA | A | 61 | 16.747 | 14.881 | 43.500 | 1.00 | 37.44 | O |
| ATOM | 366 | CB | ALA | A | 61 | 16.669 | 16.706 | 46.138 | 1.00 | 38.33 | C |
| ATOM | 367 | N | ASN | A | 62 | 17.941 | 13.927 | 45.173 | 1.00 | 35.32 | N |
| ATOM | 368 | CA | ASN | A | 62 | 17.749 | 12.557 | 44.711 | 1.00 | 33.87 | C |
| ATOM | 369 | C | ASN | A | 62 | 16.283 | 12.160 | 44.575 | 1.00 | 33.26 | C |
| ATOM | 370 | O | ASN | A | 62 | 15.938 | 11.369 | 43.700 | 1.00 | 32.65 | O |
| ATOM | 371 | CB | ASN | A | 62 | 18.504 | 11.575 | 45.613 | 1.00 | 33.16 | C |
| ATOM | 372 | CG | ASN | A | 62 | 20.007 | 11.672 | 45.443 | 1.00 | 31.36 | C |
| ATOM | 373 | OD1 | ASN | A | 62 | 20.495 | 12.030 | 44.378 | 1.00 | 29.55 | O |
| ATOM | 374 | ND2 | ASN | A | 62 | 20.748 | 11.355 | 46.497 | 1.00 | 30.76 | N |
| ATOM | 375 | N | LYS | A | 63 | 15.433 | 12.716 | 45.439 | 1.00 | 32.87 | N |
| ATOM | 376 | CA | LYS | A | 63 | 13.982 | 12.535 | 45.347 | 1.00 | 32.57 | C |
| ATOM | 377 | C | LYS | A | 63 | 13.442 | 13.039 | 44.003 | 1.00 | 31.95 | C |
| ATOM | 378 | O | LYS | A | 63 | 12.674 | 12.340 | 43.341 | 1.00 | 31.76 | O |
| ATOM | 379 | CB | LYS | A | 63 | 13.274 | 13.242 | 46.508 | 1.00 | 32.63 | C |
| ATOM | 380 | CG | LYS | A | 63 | 11.799 | 12.903 | 46.642 | 1.00 | 33.34 | C |
| ATOM | 381 | CD | LYS | A | 63 | 10.922 | 14.062 | 46.192 | 1.00 | 34.80 | C |
| ATOM | 382 | CE | LYS | A | 63 | 9.510 | 13.959 | 46.760 | 1.00 | 35.00 | C |
| ATOM | 383 | NZ | LYS | A | 63 | 8.667 | 12.959 | 46.037 | 1.00 | 34.41 | N |
| ATOM | 384 | N | GLU | A | 64 | 13.866 | 14.243 | 43.611 | 1.00 | 31.60 | N |
| ATOM | 385 | CA | GLU | A | 64 | 13.473 | 14.856 | 42.335 | 1.00 | 31.29 | C |
| ATOM | 386 | C | GLU | A | 64 | 13.942 | 14.008 | 41.151 | 1.00 | 30.22 | C |
| ATOM | 387 | O | GLU | A | 64 | 13.179 | 13.774 | 40.211 | 1.00 | 30.16 | O |
| ATOM | 388 | CB | GLU | A | 64 | 14.009 | 16.297 | 42.217 | 1.00 | 31.90 | C |
| ATOM | 389 | CG | GLU | A | 64 | 13.717 | 17.185 | 43.426 | 1.00 | 34.19 | C |
| ATOM | 390 | CD | GLU | A | 64 | 14.354 | 18.563 | 43.325 | 1.00 | 36.57 | C |
| ATOM | 391 | OE1 | GLU | A | 64 | 15.584 | 18.684 | 43.535 | 1.00 | 37.30 | O |
| ATOM | 392 | OE2 | GLU | A | 64 | 13.621 | 19.535 | 43.044 | 1.00 | 38.23 | O |
| ATOM | 393 | N | ILE | A | 65 | 15.183 | 13.527 | 41.221 | 1.00 | 29.20 | N |
| ATOM | 394 | CA | ILE | A | 65 | 15.747 | 12.657 | 40.185 | 1.00 | 28.46 | C |
| ATOM | 395 | C | ILE | A | 65 | 14.981 | 11.335 | 40.055 | 1.00 | 27.91 | C |
| ATOM | 396 | O | ILE | A | 65 | 14.675 | 10.903 | 38.942 | 1.00 | 27.51 | O |
| ATOM | 397 | CB | ILE | A | 65 | 17.264 | 12.419 | 40.417 | 1.00 | 28.67 | C |
| ATOM | 398 | CG1 | ILE | A | 65 | 18.038 | 13.741 | 40.273 | 1.00 | 28.41 | C |
| ATOM | 399 | CD1 | ILE | A | 65 | 19.425 | 13.732 | 40.880 | 1.00 | 27.82 | C |
| ATOM | 400 | CG2 | ILE | A | 65 | 17.811 | 11.343 | 39.452 | 1.00 | 28.82 | C |
| ATOM | 401 | N | LEU | A | 66 | 14.651 | 10.711 | 41.184 | 1.00 | 27.42 | N |
| ATOM | 402 | CA | LEU | A | 66 | 13.949 | 9.422 | 41.159 | 1.00 | 27.61 | C |
| ATOM | 403 | C | LEU | A | 66 | 12.507 | 9.539 | 40.657 | 1.00 | 27.13 | C |
| ATOM | 404 | O | LEU | A | 66 | 12.043 | 8.676 | 39.907 | 1.00 | 27.11 | O |
| ATOM | 405 | CB | LEU | A | 66 | 14.007 | 8.712 | 42.516 | 1.00 | 27.31 | C |
| ATOM | 406 | CG | LEU | A | 66 | 15.374 | 8.154 | 42.929 | 1.00 | 27.72 | C |
| ATOM | 407 | CD1 | LEU | A | 66 | 15.389 | 7.907 | 44.416 | 1.00 | 27.05 | C |
| ATOM | 408 | CD2 | LEU | A | 66 | 15.748 | 6.881 | 42.168 | 1.00 | 27.26 | C |
| ATOM | 409 | N | ASP | A | 67 | 11.822 | 10.612 | 41.056 | 1.00 | 27.04 | N |
| ATOM | 410 | CA | ASP | A | 67 | 10.485 | 10.940 | 40.539 | 1.00 | 26.69 | C |
| ATOM | 411 | C | ASP | A | 67 | 10.494 | 11.086 | 39.018 | 1.00 | 25.69 | C |
| ATOM | 412 | O | ASP | A | 67 | 9.629 | 10.548 | 38.332 | 1.00 | 25.85 | O |
| ATOM | 413 | CB | ASP | A | 67 | 9.971 | 12.239 | 41.162 | 1.00 | 27.16 | C |
| ATOM | 414 | CG | ASP | A | 67 | 9.361 | 12.032 | 42.539 | 1.00 | 29.29 | C |

FIG. 5G

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 415 | OD1 | ASP | A | 67 | 8.972 | 10.886 | 42.875 | 1.00 | 29.74 | O |
| ATOM | 416 | OD2 | ASP | A | 67 | 9.231 | 12.974 | 43.354 | 1.00 | 30.45 | O |
| ATOM | 417 | N | GLU | A | 68 | 11.468 | 11.832 | 38.508 | 1.00 | 24.70 | N |
| ATOM | 418 | CA | GLU | A | 68 | 11.726 | 11.918 | 37.073 | 1.00 | 24.03 | C |
| ATOM | 419 | C | GLU | A | 68 | 11.972 | 10.533 | 36.470 | 1.00 | 23.27 | C |
| ATOM | 420 | O | GLU | A | 68 | 11.312 | 10.152 | 35.509 | 1.00 | 23.42 | O |
| ATOM | 421 | CB | GLU | A | 68 | 12.923 | 12.834 | 36.801 | 1.00 | 23.85 | C |
| ATOM | 422 | CG | GLU | A | 68 | 12.592 | 14.319 | 36.917 | 1.00 | 25.07 | C |
| ATOM | 423 | N | ALA | A | 69 | 12.896 | 9.776 | 37.064 | 1.00 | 22.26 | N |
| ATOM | 424 | CA | ALA | A | 69 | 13.280 | 8.456 | 36.557 | 1.00 | 21.45 | C |
| ATOM | 425 | C | ALA | A | 69 | 12.112 | 7.455 | 36.455 | 1.00 | 21.00 | C |
| ATOM | 426 | O | ALA | A | 69 | 12.124 | 6.560 | 35.607 | 1.00 | 20.28 | O |
| ATOM | 427 | CB | ALA | A | 69 | 14.426 | 7.876 | 37.396 | 1.00 | 21.07 | C |
| ATOM | 428 | N | TYR | A | 70 | 11.115 | 7.612 | 37.325 | 1.00 | 20.80 | N |
| ATOM | 429 | CA | TYR | A | 70 | 9.941 | 6.744 | 37.324 | 1.00 | 20.38 | C |
| ATOM | 430 | C | TYR | A | 70 | 9.068 | 6.998 | 36.099 | 1.00 | 19.92 | C |
| ATOM | 431 | O | TYR | A | 70 | 8.530 | 6.061 | 35.499 | 1.00 | 19.47 | O |
| ATOM | 432 | CB | TYR | A | 70 | 9.127 | 6.937 | 38.608 | 1.00 | 20.99 | C |
| ATOM | 433 | N | VAL | A | 71 | 8.942 | 8.269 | 35.723 | 1.00 | 19.60 | N |
| ATOM | 434 | CA | VAL | A | 71 | 8.214 | 8.643 | 34.509 | 1.00 | 19.21 | C |
| ATOM | 435 | C | VAL | A | 71 | 8.933 | 8.051 | 33.287 | 1.00 | 19.25 | C |
| ATOM | 436 | O | VAL | A | 71 | 8.305 | 7.430 | 32.434 | 1.00 | 19.48 | O |
| ATOM | 437 | CB | VAL | A | 71 | 8.023 | 10.184 | 34.414 | 1.00 | 19.46 | C |
| ATOM | 438 | CG1 | VAL | A | 71 | 7.482 | 10.609 | 33.047 | 1.00 | 19.14 | C |
| ATOM | 439 | CG2 | VAL | A | 71 | 7.092 | 10.683 | 35.550 | 1.00 | 18.30 | C |
| ATOM | 440 | N | MET | A | 72 | 10.253 | 8.195 | 33.245 | 1.00 | 19.41 | N |
| ATOM | 441 | CA | MET | A | 72 | 11.070 | 7.693 | 32.135 | 1.00 | 20.02 | C |
| ATOM | 442 | C | MET | A | 72 | 11.009 | 6.176 | 32.013 | 1.00 | 20.27 | C |
| ATOM | 443 | O | MET | A | 72 | 11.137 | 5.632 | 30.910 | 1.00 | 19.98 | O |
| ATOM | 444 | CB | MET | A | 72 | 12.529 | 8.125 | 32.307 | 1.00 | 19.83 | C |
| ATOM | 445 | CG | MET | A | 72 | 12.760 | 9.615 | 32.117 | 1.00 | 20.80 | C |
| ATOM | 446 | SD | MET | A | 72 | 14.129 | 10.241 | 33.089 | 1.00 | 22.57 | S |
| ATOM | 447 | CE | MET | A | 72 | 15.484 | 9.837 | 32.011 | 1.00 | 20.49 | C |
| ATOM | 448 | N | ALA | A | 73 | 10.831 | 5.515 | 33.157 | 1.00 | 20.62 | N |
| ATOM | 449 | CA | ALA | A | 73 | 10.760 | 4.065 | 33.249 | 1.00 | 21.88 | C |
| ATOM | 450 | C | ALA | A | 73 | 9.353 | 3.539 | 32.973 | 1.00 | 22.79 | C |
| ATOM | 451 | O | ALA | A | 73 | 9.170 | 2.338 | 32.767 | 1.00 | 23.39 | O |
| ATOM | 452 | CB | ALA | A | 73 | 11.225 | 3.611 | 34.622 | 1.00 | 22.42 | C |
| ATOM | 453 | N | SER | A | 74 | 8.372 | 4.444 | 32.974 | 1.00 | 22.94 | N |
| ATOM | 454 | CA | SER | A | 74 | 6.981 | 4.114 | 32.677 | 1.00 | 22.93 | C |
| ATOM | 455 | C | SER | A | 74 | 6.666 | 4.201 | 31.183 | 1.00 | 23.31 | C |
| ATOM | 456 | O | SER | A | 74 | 5.573 | 3.811 | 30.757 | 1.00 | 23.60 | O |
| ATOM | 457 | CB | SER | A | 74 | 6.040 | 5.040 | 33.452 | 1.00 | 23.30 | C |
| ATOM | 458 | OG | SER | A | 74 | 5.894 | 6.301 | 32.805 | 1.00 | 22.24 | O |
| ATOM | 459 | N | VAL | A | 75 | 7.616 | 4.713 | 30.398 | 1.00 | 23.17 | N |
| ATOM | 460 | CA | VAL | A | 75 | 7.438 | 4.856 | 28.951 | 1.00 | 22.82 | C |
| ATOM | 461 | C | VAL | A | 75 | 7.548 | 3.496 | 28.264 | 1.00 | 22.84 | C |
| ATOM | 462 | O | VAL | A | 75 | 8.611 | 2.887 | 28.224 | 1.00 | 23.12 | O |
| ATOM | 463 | CB | VAL | A | 75 | 8.428 | 5.885 | 28.331 | 1.00 | 23.28 | C |
| ATOM | 464 | CG1 | VAL | A | 75 | 8.446 | 5.776 | 26.813 | 1.00 | 22.51 | C |
| ATOM | 465 | CG2 | VAL | A | 75 | 8.067 | 7.308 | 28.746 | 1.00 | 21.50 | C |
| ATOM | 466 | N | ASP | A | 76 | 6.427 | 3.034 | 27.720 | 1.00 | 22.57 | N |
| ATOM | 467 | CA | ASP | A | 76 | 6.309 | 1.693 | 27.173 | 1.00 | 21.55 | C |
| ATOM | 468 | C | ASP | A | 76 | 5.786 | 1.788 | 25.747 | 1.00 | 20.62 | C |
| ATOM | 469 | O | ASP | A | 76 | 4.584 | 1.803 | 25.521 | 1.00 | 19.62 | O |
| ATOM | 470 | CB | ASP | A | 76 | 5.378 | 0.861 | 28.068 | 1.00 | 22.23 | C |
| ATOM | 471 | CG | ASP | A | 76 | 5.120 | -0.550 | 27.526 | 1.00 | 24.21 | C |
| ATOM | 472 | OD1 | ASP | A | 76 | 6.014 | -1.140 | 26.878 | 1.00 | 24.17 | O |
| ATOM | 473 | OD2 | ASP | A | 76 | 4.039 | -1.152 | 27.719 | 1.00 | 26.10 | O |
| ATOM | 474 | N | ASN | A | 77 | 6.714 | 1.872 | 24.791 | 1.00 | 20.02 | N |

FIG. 5H

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 475 | CA | ASN | A | 77 | 6.391 | 1.994 | 23.371 | 1.00 | 18.19 | C |
| ATOM | 476 | C | ASN | A | 77 | 7.530 | 1.436 | 22.523 | 1.00 | 17.44 | C |
| ATOM | 477 | O | ASN | A | 77 | 8.688 | 1.648 | 22.847 | 1.00 | 17.56 | O |
| ATOM | 478 | CB | ASN | A | 77 | 6.136 | 3.462 | 23.007 | 1.00 | 18.47 | C |
| ATOM | 479 | CG | ASN | A | 77 | 5.657 | 3.636 | 21.579 | 1.00 | 17.62 | C |
| ATOM | 480 | OD1 | ASN | A | 77 | 6.447 | 3.827 | 20.662 | 1.00 | 18.29 | O |
| ATOM | 481 | ND2 | ASN | A | 77 | 4.361 | 3.542 | 21.387 | 1.00 | 18.96 | N |
| ATOM | 482 | N | PRO | A | 78 | 7.214 | 0.713 | 21.449 | 1.00 | 16.86 | N |
| ATOM | 483 | CA | PRO | A | 78 | 8.250 | 0.094 | 20.612 | 1.00 | 16.27 | C |
| ATOM | 484 | C | PRO | A | 78 | 9.247 | 1.093 | 20.020 | 1.00 | 16.15 | C |
| ATOM | 485 | O | PRO | A | 78 | 10.343 | 0.677 | 19.660 | 1.00 | 15.86 | O |
| ATOM | 486 | CB | PRO | A | 78 | 7.444 | -0.575 | 19.492 | 1.00 | 16.03 | C |
| ATOM | 487 | CG | PRO | A | 78 | 6.119 | -0.815 | 20.098 | 1.00 | 17.12 | C |
| ATOM | 488 | CD | PRO | A | 78 | 5.857 | 0.399 | 20.958 | 1.00 | 16.41 | C |
| ATOM | 489 | N | HIS | A | 79 | 8.886 | 2.374 | 19.946 | 1.00 | 15.40 | N |
| ATOM | 490 | CA | HIS | A | 79 | 9.760 | 3.365 | 19.333 | 1.00 | 15.22 | C |
| ATOM | 491 | C | HIS | A | 79 | 10.233 | 4.450 | 20.297 | 1.00 | 15.68 | C |
| ATOM | 492 | O | HIS | A | 79 | 10.677 | 5.519 | 19.863 | 1.00 | 15.57 | O |
| ATOM | 493 | CB | HIS | A | 79 | 9.092 | 3.955 | 18.080 | 1.00 | 15.62 | C |
| ATOM | 494 | CG | HIS | A | 79 | 8.611 | 2.909 | 17.121 | 1.00 | 15.43 | C |
| ATOM | 495 | ND1 | HIS | A | 79 | 9.474 | 2.093 | 16.420 | 1.00 | 16.86 | N |
| ATOM | 496 | CE1 | HIS | A | 79 | 8.777 | 1.247 | 15.683 | 1.00 | 16.30 | C |
| ATOM | 497 | NE2 | HIS | A | 79 | 7.492 | 1.477 | 15.891 | 1.00 | 16.57 | N |
| ATOM | 498 | CD2 | HIS | A | 79 | 7.361 | 2.501 | 16.798 | 1.00 | 15.31 | C |
| ATOM | 499 | N | VAL | A | 80 | 10.135 | 4.181 | 21.602 | 1.00 | 15.49 | N |
| ATOM | 500 | CA | VAL | A | 80 | 10.721 | 5.065 | 22.609 | 1.00 | 16.60 | C |
| ATOM | 501 | C | VAL | A | 80 | 11.506 | 4.255 | 23.635 | 1.00 | 17.50 | C |
| ATOM | 502 | O | VAL | A | 80 | 11.006 | 3.268 | 24.169 | 1.00 | 18.27 | O |
| ATOM | 503 | CB | VAL | A | 80 | 9.679 | 5.995 | 23.325 | 1.00 | 16.27 | C |
| ATOM | 504 | CG1 | VAL | A | 80 | 10.387 | 7.097 | 24.114 | 1.00 | 14.48 | C |
| ATOM | 505 | CG2 | VAL | A | 80 | 8.725 | 6.640 | 22.335 | 1.00 | 16.07 | C |
| ATOM | 506 | N | CYS | A | 81 | 12.742 | 4.667 | 23.895 | 1.00 | 18.30 | N |
| ATOM | 507 | CA | CYS | A | 81 | 13.580 | 3.985 | 24.873 | 1.00 | 19.69 | C |
| ATOM | 508 | C | CYS | A | 81 | 13.018 | 4.154 | 26.275 | 1.00 | 19.91 | C |
| ATOM | 509 | O | CYS | A | 81 | 12.730 | 5.276 | 26.707 | 1.00 | 20.18 | O |
| ATOM | 510 | CB | CYS | A | 81 | 15.003 | 4.531 | 24.822 | 1.00 | 20.00 | C |
| ATOM | 511 | SG | CYS | A | 81 | 15.814 | 4.263 | 23.228 | 1.00 | 23.58 | S |
| ATOM | 512 | N | ARG | A | 82 | 12.841 | 3.044 | 26.985 | 1.00 | 20.26 | N |
| ATOM | 513 | CA | ARG | A | 82 | 12.472 | 3.139 | 28.388 | 1.00 | 20.30 | C |
| ATOM | 514 | C | ARG | A | 82 | 13.690 | 3.034 | 29.290 | 1.00 | 19.96 | C |
| ATOM | 515 | O | ARG | A | 82 | 14.624 | 2.295 | 29.009 | 1.00 | 19.48 | O |
| ATOM | 516 | CB | ARG | A | 82 | 11.384 | 2.137 | 28.790 | 1.00 | 20.37 | C |
| ATOM | 517 | CG | ARG | A | 82 | 11.583 | 0.694 | 28.375 | 1.00 | 22.08 | C |
| ATOM | 518 | CD | ARG | A | 82 | 10.731 | -0.305 | 29.198 | 1.00 | 22.79 | C |
| ATOM | 519 | NE | ARG | A | 82 | 10.607 | 0.134 | 30.585 | 1.00 | 23.81 | N |
| ATOM | 520 | CZ | ARG | A | 82 | 10.972 | -0.573 | 31.651 | 1.00 | 24.16 | C |
| ATOM | 521 | NH1 | ARG | A | 82 | 10.831 | -0.052 | 32.865 | 1.00 | 23.28 | N |
| ATOM | 522 | NH2 | ARG | A | 82 | 11.465 | -1.798 | 31.515 | 1.00 | 24.76 | N |
| ATOM | 523 | N | LEU | A | 83 | 13.674 | 3.812 | 30.361 | 1.00 | 19.66 | N |
| ATOM | 524 | CA | LEU | A | 83 | 14.679 | 3.694 | 31.393 | 1.00 | 19.40 | C |
| ATOM | 525 | C | LEU | A | 83 | 14.452 | 2.359 | 32.110 | 1.00 | 19.16 | C |
| ATOM | 526 | O | LEU | A | 83 | 13.349 | 2.087 | 32.567 | 1.00 | 19.07 | O |
| ATOM | 527 | CB | LEU | A | 83 | 14.591 | 4.886 | 32.371 | 1.00 | 18.78 | C |
| ATOM | 528 | CG | LEU | A | 83 | 15.713 | 4.943 | 33.418 | 1.00 | 18.61 | C |
| ATOM | 529 | CD1 | LEU | A | 83 | 17.054 | 4.993 | 32.737 | 1.00 | 17.65 | C |
| ATOM | 530 | CD2 | LEU | A | 83 | 15.569 | 6.108 | 34.392 | 1.00 | 18.78 | C |
| ATOM | 531 | N | LEU | A | 84 | 15.479 | 1.515 | 32.171 | 1.00 | 19.27 | N |
| ATOM | 532 | CA | LEU | A | 84 | 15.361 | 0.260 | 32.907 | 1.00 | 19.61 | C |
| ATOM | 533 | C | LEU | A | 84 | 15.807 | 0.471 | 34.347 | 1.00 | 19.11 | C |
| ATOM | 534 | O | LEU | A | 84 | 15.124 | 0.067 | 35.287 | 1.00 | 19.28 | O |

FIG. 5I

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 535 | CB | LEU | A | 84 | 16.189 | -0.870 | 32.262 | 1.00 | 19.77 | C |
| ATOM | 536 | CG | LEU | A | 84 | 15.880 | -1.353 | 30.845 | 1.00 | 21.49 | C |
| ATOM | 537 | CD1 | LEU | A | 84 | 16.915 | -2.373 | 30.424 | 1.00 | 22.18 | C |
| ATOM | 538 | CD2 | LEU | A | 84 | 14.481 | -1.930 | 30.708 | 1.00 | 22.51 | C |
| ATOM | 539 | N | GLY | A | 85 | 16.962 | 1.104 | 34.509 | 1.00 | 18.77 | N |
| ATOM | 540 | CA | GLY | A | 85 | 17.590 | 1.215 | 35.809 | 1.00 | 18.72 | C |
| ATOM | 541 | C | GLY | A | 85 | 18.286 | 2.531 | 36.053 | 1.00 | 18.38 | C |
| ATOM | 542 | O | GLY | A | 85 | 18.658 | 3.235 | 35.115 | 1.00 | 17.12 | O |
| ATOM | 543 | N | ILE | A | 86 | 18.440 | 2.855 | 37.336 | 1.00 | 19.45 | N |
| ATOM | 544 | CA | ILE | A | 86 | 19.195 | 4.021 | 37.785 | 1.00 | 20.39 | C |
| ATOM | 545 | C | ILE | A | 86 | 20.125 | 3.611 | 38.930 | 1.00 | 21.45 | C |
| ATOM | 546 | O | ILE | A | 86 | 19.751 | 2.830 | 39.805 | 1.00 | 21.92 | O |
| ATOM | 547 | CB | ILE | A | 86 | 18.235 | 5.196 | 38.183 | 1.00 | 20.35 | C |
| ATOM | 548 | CG1 | ILE | A | 86 | 19.007 | 6.491 | 38.463 | 1.00 | 19.99 | C |
| ATOM | 549 | CD1 | ILE | A | 86 | 18.243 | 7.731 | 38.107 | 1.00 | 18.21 | C |
| ATOM | 550 | CG2 | ILE | A | 86 | 17.335 | 4.827 | 39.368 | 1.00 | 20.52 | C |
| ATOM | 551 | N | CYS | A | 87 | 21.352 | 4.114 | 38.896 | 1.00 | 22.72 | N |
| ATOM | 552 | CA | CYS | A | 87 | 22.290 | 3.933 | 39.995 | 1.00 | 23.21 | C |
| ATOM | 553 | C | CYS | A | 87 | 22.778 | 5.301 | 40.444 | 1.00 | 23.80 | C |
| ATOM | 554 | O | CYS | A | 87 | 23.266 | 6.091 | 39.634 | 1.00 | 23.86 | O |
| ATOM | 555 | CB | CYS | A | 87 | 23.471 | 3.059 | 39.571 | 1.00 | 23.19 | C |
| ATOM | 556 | SG | CYS | A | 87 | 24.669 | 2.712 | 40.888 | 1.00 | 23.58 | S |
| ATOM | 557 | N | LEU | A | 88 | 22.622 | 5.581 | 41.733 | 1.00 | 24.63 | N |
| ATOM | 558 | CA | LEU | A | 88 | 23.062 | 6.850 | 42.309 | 1.00 | 25.54 | C |
| ATOM | 559 | C | LEU | A | 88 | 24.330 | 6.629 | 43.127 | 1.00 | 25.98 | C |
| ATOM | 560 | O | LEU | A | 88 | 24.276 | 6.159 | 44.266 | 1.00 | 25.49 | O |
| ATOM | 561 | CB | LEU | A | 88 | 21.970 | 7.473 | 43.189 | 1.00 | 25.32 | C |
| ATOM | 562 | CG | LEU | A | 88 | 20.586 | 7.790 | 42.606 | 1.00 | 26.58 | C |
| ATOM | 563 | CD1 | LEU | A | 88 | 19.607 | 8.152 | 43.740 | 1.00 | 25.60 | C |
| ATOM | 564 | CD2 | LEU | A | 88 | 20.646 | 8.908 | 41.557 | 1.00 | 25.45 | C |
| ATOM | 565 | N | THR | A | 89 | 25.468 | 6.943 | 42.522 | 1.00 | 26.50 | N |
| ATOM | 566 | CA | THR | A | 89 | 26.744 | 6.913 | 43.218 | 1.00 | 27.70 | C |
| ATOM | 567 | C | THR | A | 89 | 27.369 | 8.308 | 43.149 | 1.00 | 28.02 | C |
| ATOM | 568 | O | THR | A | 89 | 26.653 | 9.312 | 43.193 | 1.00 | 28.36 | O |
| ATOM | 569 | CB | THR | A | 89 | 27.672 | 5.834 | 42.620 | 1.00 | 27.79 | C |
| ATOM | 570 | OG1 | THR | A | 89 | 27.458 | 5.734 | 41.204 | 1.00 | 29.61 | O |
| ATOM | 571 | CG2 | THR | A | 89 | 27.272 | 4.468 | 43.118 | 1.00 | 28.40 | C |
| ATOM | 572 | N | SER | A | 90 | 28.694 | 8.368 | 43.047 | 1.00 | 28.36 | N |
| ATOM | 573 | CA | SER | A | 90 | 29.411 | 9.613 | 42.768 | 1.00 | 28.77 | C |
| ATOM | 574 | C | SER | A | 90 | 28.861 | 10.319 | 41.530 | 1.00 | 28.51 | C |
| ATOM | 575 | O | SER | A | 90 | 28.874 | 11.546 | 41.446 | 1.00 | 29.21 | O |
| ATOM | 576 | CB | SER | A | 90 | 30.895 | 9.321 | 42.571 | 1.00 | 28.96 | C |
| ATOM | 577 | OG | SER | A | 90 | 31.140 | 7.923 | 42.627 | 1.00 | 30.78 | O |
| ATOM | 578 | N | THR | A | 91 | 28.390 | 9.528 | 40.571 | 1.00 | 27.93 | N |
| ATOM | 579 | CA | THR | A | 91 | 27.723 | 10.034 | 39.382 | 1.00 | 26.94 | C |
| ATOM | 580 | C | THR | A | 91 | 26.376 | 9.350 | 39.296 | 1.00 | 26.44 | C |
| ATOM | 581 | O | THR | A | 91 | 26.204 | 8.244 | 39.821 | 1.00 | 26.63 | O |
| ATOM | 582 | CB | THR | A | 91 | 28.533 | 9.684 | 38.104 | 1.00 | 27.12 | C |
| ATOM | 583 | OG1 | THR | A | 91 | 28.800 | 8.277 | 38.078 | 1.00 | 26.60 | O |
| ATOM | 584 | CG2 | THR | A | 91 | 29.933 | 10.314 | 38.127 | 1.00 | 26.50 | C |
| ATOM | 585 | N | VAL | A | 92 | 25.425 | 10.009 | 38.637 | 1.00 | 25.44 | N |
| ATOM | 586 | CA | VAL | A | 92 | 24.182 | 9.366 | 38.231 | 1.00 | 24.57 | C |
| ATOM | 587 | C | VAL | A | 92 | 24.460 | 8.515 | 36.983 | 1.00 | 24.00 | C |
| ATOM | 588 | O | VAL | A | 92 | 25.054 | 8.999 | 36.023 | 1.00 | 23.88 | O |
| ATOM | 589 | CB | VAL | A | 92 | 23.071 | 10.404 | 37.946 | 1.00 | 24.61 | C |
| ATOM | 590 | CG1 | VAL | A | 92 | 21.773 | 9.725 | 37.520 | 1.00 | 24.41 | C |
| ATOM | 591 | CG2 | VAL | A | 92 | 22.823 | 11.269 | 39.171 | 1.00 | 24.70 | C |
| ATOM | 592 | N | GLN | A | 93 | 24.056 | 7.246 | 37.015 | 1.00 | 23.07 | N |
| ATOM | 593 | CA | GLN | A | 93 | 24.162 | 6.369 | 35.847 | 1.00 | 22.58 | C |
| ATOM | 594 | C | GLN | A | 93 | 22.795 | 5.817 | 35.465 | 1.00 | 22.04 | C |

FIG. 5J

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 595 | O | GLN | A | 93 | 22.053 | 5.334 | 36.325 | 1.00 | 21.73 | O |
| ATOM | 596 | CB | GLN | A | 93 | 25.151 | 5.225 | 36.098 | 1.00 | 22.93 | C |
| ATOM | 597 | CG | GLN | A | 93 | 26.586 | 5.683 | 36.290 | 1.00 | 24.03 | C |
| ATOM | 598 | CD | GLN | A | 93 | 27.520 | 4.555 | 36.652 | 1.00 | 25.78 | C |
| ATOM | 599 | OE1 | GLN | A | 93 | 28.106 | 3.920 | 35.777 | 1.00 | 28.14 | O |
| ATOM | 600 | NE2 | GLN | A | 93 | 27.667 | 4.301 | 37.936 | 1.00 | 26.44 | N |
| ATOM | 601 | N | LEU | A | 94 | 22.456 | 5.916 | 34.179 | 1.00 | 21.75 | N |
| ATOM | 602 | CA | LEU | A | 94 | 21.175 | 5.418 | 33.674 | 1.00 | 21.57 | C |
| ATOM | 603 | C | LEU | A | 94 | 21.389 | 4.198 | 32.805 | 1.00 | 21.40 | C |
| ATOM | 604 | O | LEU | A | 94 | 22.333 | 4.154 | 32.026 | 1.00 | 20.98 | O |
| ATOM | 605 | CB | LEU | A | 94 | 20.418 | 6.496 | 32.889 | 1.00 | 21.58 | C |
| ATOM | 606 | CG | LEU | A | 94 | 20.199 | 7.878 | 33.508 | 1.00 | 21.61 | C |
| ATOM | 607 | CD1 | LEU | A | 94 | 19.322 | 8.735 | 32.596 | 1.00 | 22.05 | C |
| ATOM | 608 | CD2 | LEU | A | 94 | 19.612 | 7.803 | 34.911 | 1.00 | 20.53 | C |
| ATOM | 609 | N | ILE | A | 95 | 20.499 | 3.216 | 32.944 | 1.00 | 21.48 | N |
| ATOM | 610 | CA | ILE | A | 95 | 20.665 | 1.914 | 32.303 | 1.00 | 21.10 | C |
| ATOM | 611 | C | ILE | A | 95 | 19.498 | 1.622 | 31.350 | 1.00 | 21.34 | C |
| ATOM | 612 | O | ILE | A | 95 | 18.327 | 1.671 | 31.751 | 1.00 | 22.01 | O |
| ATOM | 613 | CB | ILE | A | 95 | 20.843 | 0.797 | 33.378 | 1.00 | 21.27 | C |
| ATOM | 614 | CG1 | ILE | A | 95 | 22.148 | 1.007 | 34.167 | 1.00 | 22.39 | C |
| ATOM | 615 | CD1 | ILE | A | 95 | 21.982 | 1.673 | 35.535 | 1.00 | 21.44 | C |
| ATOM | 616 | CG2 | ILE | A | 95 | 20.867 | -0.602 | 32.748 | 1.00 | 19.87 | C |
| ATOM | 617 | N | THR | A | 96 | 19.825 | 1.341 | 30.090 | 1.00 | 20.59 | N |
| ATOM | 618 | CA | THR | A | 96 | 18.813 | 1.072 | 29.061 | 1.00 | 21.13 | C |
| ATOM | 619 | C | THR | A | 96 | 19.181 | -0.143 | 28.219 | 1.00 | 21.31 | C |
| ATOM | 620 | O | THR | A | 96 | 20.293 | -0.672 | 28.311 | 1.00 | 21.68 | O |
| ATOM | 621 | CB | THR | A | 96 | 18.605 | 2.301 | 28.117 | 1.00 | 20.82 | C |
| ATOM | 622 | OG1 | THR | A | 96 | 19.871 | 2.759 | 27.619 | 1.00 | 20.52 | O |
| ATOM | 623 | CG2 | THR | A | 96 | 18.061 | 3.502 | 28.868 | 1.00 | 19.81 | C |
| ATOM | 624 | N | GLN | A | 97 | 18.241 | -0.576 | 27.391 | 1.00 | 21.60 | N |
| ATOM | 625 | CA | GLN | A | 97 | 18.507 | -1.619 | 26.413 | 1.00 | 21.95 | C |
| ATOM | 626 | C | GLN | A | 97 | 19.525 | -1.113 | 25.383 | 1.00 | 21.61 | C |
| ATOM | 627 | O | GLN | A | 97 | 19.402 | 0.002 | 24.872 | 1.00 | 21.52 | O |
| ATOM | 628 | CB | GLN | A | 97 | 17.201 | -2.033 | 25.729 | 1.00 | 22.65 | C |
| ATOM | 629 | CG | GLN | A | 97 | 17.345 | -3.175 | 24.729 | 1.00 | 25.42 | C |
| ATOM | 630 | CD | GLN | A | 97 | 16.024 | -3.602 | 24.125 | 1.00 | 27.64 | C |
| ATOM | 631 | OE1 | GLN | A | 97 | 15.306 | -2.789 | 23.542 | 1.00 | 30.44 | O |
| ATOM | 632 | NE2 | GLN | A | 97 | 15.702 | -4.879 | 24.253 | 1.00 | 28.73 | N |
| ATOM | 633 | N | LEU | A | 98 | 20.526 | -1.935 | 25.089 | 1.00 | 21.21 | N |
| ATOM | 634 | CA | LEU | A | 98 | 21.557 | -1.586 | 24.120 | 1.00 | 21.22 | C |
| ATOM | 635 | C | LEU | A | 98 | 20.970 | -1.528 | 22.715 | 1.00 | 20.98 | C |
| ATOM | 636 | O | LEU | A | 98 | 20.366 | -2.488 | 22.254 | 1.00 | 20.92 | O |
| ATOM | 637 | CB | LEU | A | 98 | 22.715 | -2.592 | 24.169 | 1.00 | 21.47 | C |
| ATOM | 638 | CG | LEU | A | 98 | 23.869 | -2.369 | 23.184 | 1.00 | 21.69 | C |
| ATOM | 639 | CD1 | LEU | A | 98 | 24.765 | -1.243 | 23.669 | 1.00 | 22.47 | C |
| ATOM | 640 | CD2 | LEU | A | 98 | 24.689 | -3.650 | 22.959 | 1.00 | 21.77 | C |
| ATOM | 641 | N | MET | A | 99 | 21.131 | -0.384 | 22.060 | 1.00 | 20.84 | N |
| ATOM | 642 | CA | MET | A | 99 | 20.710 | -0.211 | 20.679 | 1.00 | 20.64 | C |
| ATOM | 643 | C | MET | A | 99 | 21.974 | -0.336 | 19.848 | 1.00 | 20.57 | C |
| ATOM | 644 | O | MET | A | 99 | 22.689 | 0.646 | 19.639 | 1.00 | 20.89 | O |
| ATOM | 645 | CB | MET | A | 99 | 20.041 | 1.156 | 20.477 | 1.00 | 20.96 | C |
| ATOM | 646 | CG | MET | A | 99 | 18.836 | 1.406 | 21.382 | 1.00 | 21.84 | C |
| ATOM | 647 | SD | MET | A | 99 | 17.421 | 0.417 | 20.855 | 1.00 | 24.46 | S |
| ATOM | 648 | CE | MET | A | 99 | 16.831 | -0.214 | 22.362 | 1.00 | 23.27 | C |
| ATOM | 649 | N | PRO | A | 100 | 22.246 | -1.555 | 19.383 | 1.00 | 20.44 | N |
| ATOM | 650 | CA | PRO | A | 100 | 23.590 | -1.941 | 18.929 | 1.00 | 20.46 | C |
| ATOM | 651 | C | PRO | A | 100 | 24.080 | -1.273 | 17.648 | 1.00 | 20.46 | C |
| ATOM | 652 | O | PRO | A | 100 | 25.259 | -1.373 | 17.334 | 1.00 | 21.31 | O |
| ATOM | 653 | CB | PRO | A | 100 | 23.465 | -3.455 | 18.724 | 1.00 | 20.75 | C |
| ATOM | 654 | CG | PRO | A | 100 | 22.030 | -3.683 | 18.442 | 1.00 | 20.42 | C |

FIG. 5K

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 655 | CD | PRO | A | 100 | 21.282 | -2.665 | 19.259 | 1.00 | 20.01 | C |
| ATOM | 656 | N | PHE | A | 101 | 23.200 | -0.600 | 16.925 | 1.00 | 20.55 | N |
| ATOM | 657 | CA | PHE | A | 101 | 23.598 | 0.075 | 15.694 | 1.00 | 19.71 | C |
| ATOM | 658 | C | PHE | A | 101 | 23.906 | 1.557 | 15.917 | 1.00 | 19.31 | C |
| ATOM | 659 | O | PHE | A | 101 | 24.315 | 2.251 | 14.987 | 1.00 | 19.85 | O |
| ATOM | 660 | CB | PHE | A | 101 | 22.531 | -0.112 | 14.610 | 1.00 | 19.90 | C |
| ATOM | 661 | CG | PHE | A | 101 | 22.474 | -1.507 | 14.040 | 1.00 | 18.56 | C |
| ATOM | 662 | CD1 | PHE | A | 101 | 23.169 | -1.824 | 12.883 | 1.00 | 19.54 | C |
| ATOM | 663 | CE1 | PHE | A | 101 | 23.119 | -3.114 | 12.337 | 1.00 | 20.06 | C |
| ATOM | 664 | CZ | PHE | A | 101 | 22.360 | -4.098 | 12.957 | 1.00 | 21.11 | C |
| ATOM | 665 | CE2 | PHE | A | 101 | 21.653 | -3.789 | 14.129 | 1.00 | 21.19 | C |
| ATOM | 666 | CD2 | PHE | A | 101 | 21.715 | -2.493 | 14.654 | 1.00 | 19.92 | C |
| ATOM | 667 | N | GLY | A | 102 | 23.724 | 2.029 | 17.149 | 1.00 | 18.54 | N |
| ATOM | 668 | CA | GLY | A | 102 | 24.049 | 3.399 | 17.509 | 1.00 | 18.28 | C |
| ATOM | 669 | C | GLY | A | 102 | 22.976 | 4.405 | 17.128 | 1.00 | 18.17 | C |
| ATOM | 670 | O | GLY | A | 102 | 21.804 | 4.045 | 16.960 | 1.00 | 17.69 | O |
| ATOM | 671 | N | CYS | A | 103 | 23.364 | 5.672 | 16.990 | 1.00 | 17.96 | N |
| ATOM | 672 | CA | CYS | A | 103 | 22.384 | 6.703 | 16.660 | 1.00 | 18.60 | C |
| ATOM | 673 | C | CYS | A | 103 | 22.111 | 6.792 | 15.160 | 1.00 | 18.16 | C |
| ATOM | 674 | O | CYS | A | 103 | 22.958 | 6.436 | 14.332 | 1.00 | 17.63 | O |
| ATOM | 675 | CB | CYS | A | 103 | 22.705 | 8.056 | 17.314 | 1.00 | 18.88 | C |
| ATOM | 676 | SG | CYS | A | 103 | 23.933 | 9.125 | 16.540 | 1.00 | 23.76 | S |
| ATOM | 677 | N | LEU | A | 104 | 20.899 | 7.225 | 14.824 | 1.00 | 18.08 | N |
| ATOM | 678 | CA | LEU | A | 104 | 20.456 | 7.283 | 13.432 | 1.00 | 18.04 | C |
| ATOM | 679 | C | LEU | A | 104 | 21.243 | 8.286 | 12.604 | 1.00 | 17.84 | C |
| ATOM | 680 | O | LEU | A | 104 | 21.523 | 8.039 | 11.436 | 1.00 | 17.15 | O |
| ATOM | 681 | CB | LEU | A | 104 | 18.954 | 7.567 | 13.350 | 1.00 | 18.23 | C |
| ATOM | 682 | CG | LEU | A | 104 | 18.217 | 7.360 | 12.021 | 1.00 | 17.77 | C |
| ATOM | 683 | CD1 | LEU | A | 104 | 18.632 | 6.090 | 11.306 | 1.00 | 18.61 | C |
| ATOM | 684 | CD2 | LEU | A | 104 | 16.715 | 7.389 | 12.264 | 1.00 | 17.10 | C |
| ATOM | 685 | N | LEU | A | 105 | 21.611 | 9.409 | 13.217 | 1.00 | 18.13 | N |
| ATOM | 686 | CA | LEU | A | 105 | 22.395 | 10.428 | 12.525 | 1.00 | 18.51 | C |
| ATOM | 687 | C | LEU | A | 105 | 23.710 | 9.851 | 11.989 | 1.00 | 18.73 | C |
| ATOM | 688 | O | LEU | A | 105 | 24.024 | 10.026 | 10.814 | 1.00 | 18.31 | O |
| ATOM | 689 | CB | LEU | A | 105 | 22.679 | 11.626 | 13.438 | 1.00 | 18.21 | C |
| ATOM | 690 | CG | LEU | A | 105 | 23.532 | 12.745 | 12.828 | 1.00 | 17.88 | C |
| ATOM | 691 | CD1 | LEU | A | 105 | 22.832 | 13.392 | 11.628 | 1.00 | 17.11 | C |
| ATOM | 692 | CD2 | LEU | A | 105 | 23.866 | 13.790 | 13.882 | 1.00 | 18.01 | C |
| ATOM | 693 | N | ASP | A | 106 | 24.468 | 9.177 | 12.855 | 1.00 | 18.92 | N |
| ATOM | 694 | CA | ASP | A | 106 | 25.702 | 8.505 | 12.446 | 1.00 | 19.98 | C |
| ATOM | 695 | C | ASP | A | 106 | 25.411 | 7.402 | 11.450 | 1.00 | 19.53 | C |
| ATOM | 696 | O | ASP | A | 106 | 26.184 | 7.183 | 10.513 | 1.00 | 19.02 | O |
| ATOM | 697 | CB | ASP | A | 106 | 26.436 | 7.907 | 13.648 | 1.00 | 20.21 | C |
| ATOM | 698 | CG | ASP | A | 106 | 27.046 | 8.959 | 14.529 | 1.00 | 22.69 | C |
| ATOM | 699 | OD1 | ASP | A | 106 | 27.205 | 10.117 | 14.076 | 1.00 | 25.34 | O |
| ATOM | 700 | OD2 | ASP | A | 106 | 27.389 | 8.727 | 15.701 | 1.00 | 25.14 | O |
| ATOM | 701 | N | TYR | A | 107 | 24.294 | 6.712 | 11.660 | 1.00 | 19.26 | N |
| ATOM | 702 | CA | TYR | A | 107 | 23.916 | 5.633 | 10.768 | 1.00 | 20.05 | C |
| ATOM | 703 | C | TYR | A | 107 | 23.729 | 6.104 | 9.324 | 1.00 | 20.13 | C |
| ATOM | 704 | O | TYR | A | 107 | 24.266 | 5.490 | 8.404 | 1.00 | 19.85 | O |
| ATOM | 705 | CB | TYR | A | 107 | 22.660 | 4.907 | 11.258 | 1.00 | 19.83 | C |
| ATOM | 706 | CG | TYR | A | 107 | 22.399 | 3.660 | 10.462 | 1.00 | 20.23 | C |
| ATOM | 707 | CD1 | TYR | A | 107 | 23.043 | 2.459 | 10.775 | 1.00 | 19.74 | C |
| ATOM | 708 | CE1 | TYR | A | 107 | 22.812 | 1.319 | 10.030 | 1.00 | 20.62 | C |
| ATOM | 709 | CZ | TYR | A | 107 | 21.948 | 1.381 | 8.940 | 1.00 | 20.32 | C |
| ATOM | 710 | OH | TYR | A | 107 | 21.701 | 0.268 | 8.192 | 1.00 | 20.73 | O |
| ATOM | 711 | CE2 | TYR | A | 107 | 21.313 | 2.558 | 8.604 | 1.00 | 20.02 | C |
| ATOM | 712 | CD2 | TYR | A | 107 | 21.549 | 3.689 | 9.358 | 1.00 | 20.45 | C |
| ATOM | 713 | N | VAL | A | 108 | 22.960 | 7.178 | 9.139 | 1.00 | 20.55 | N |
| ATOM | 714 | CA | VAL | A | 108 | 22.677 | 7.702 | 7.803 | 1.00 | 20.82 | C |

FIG. 5L

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 715 | C | VAL | A | 108 | 23.940 | 8.266 | 7.147 | 1.00 | 21.24 | C |
| ATOM | 716 | O | VAL | A | 108 | 24.123 | 8.117 | 5.941 | 1.00 | 21.02 | O |
| ATOM | 717 | CB | VAL | A | 108 | 21.497 | 8.721 | 7.771 | 1.00 | 21.20 | C |
| ATOM | 718 | CG1 | VAL | A | 108 | 20.225 | 8.101 | 8.345 | 1.00 | 20.62 | C |
| ATOM | 719 | CG2 | VAL | A | 108 | 21.847 | 10.033 | 8.495 | 1.00 | 21.22 | C |
| ATOM | 720 | N | ARG | A | 109 | 24.813 | 8.880 | 7.950 | 1.00 | 21.24 | N |
| ATOM | 721 | CA | ARG | A | 109 | 26.085 | 9.413 | 7.458 | 1.00 | 21.59 | C |
| ATOM | 722 | C | ARG | A | 109 | 27.042 | 8.321 | 6.973 | 1.00 | 22.33 | C |
| ATOM | 723 | O | ARG | A | 109 | 27.792 | 8.519 | 6.005 | 1.00 | 21.98 | O |
| ATOM | 724 | CB | ARG | A | 109 | 26.777 | 10.224 | 8.543 | 1.00 | 21.05 | C |
| ATOM | 725 | CG | ARG | A | 109 | 26.213 | 11.597 | 8.738 | 1.00 | 20.31 | C |
| ATOM | 726 | CD | ARG | A | 109 | 26.821 | 12.343 | 9.909 | 1.00 | 19.56 | C |
| ATOM | 727 | NE | ARG | A | 109 | 26.153 | 13.624 | 10.073 | 1.00 | 21.62 | N |
| ATOM | 728 | CZ | ARG | A | 109 | 26.400 | 14.488 | 11.038 | 1.00 | 21.72 | C |
| ATOM | 729 | NH1 | ARG | A | 109 | 27.318 | 14.221 | 11.956 | 1.00 | 22.70 | N |
| ATOM | 730 | NH2 | ARG | A | 109 | 25.717 | 15.622 | 11.091 | 1.00 | 21.34 | N |
| ATOM | 731 | N | GLU | A | 110 | 27.017 | 7.183 | 7.664 | 1.00 | 23.09 | N |
| ATOM | 732 | CA | GLU | A | 110 | 27.893 | 6.055 | 7.361 | 1.00 | 24.21 | C |
| ATOM | 733 | C | GLU | A | 110 | 27.354 | 5.157 | 6.241 | 1.00 | 25.04 | C |
| ATOM | 734 | O | GLU | A | 110 | 28.128 | 4.645 | 5.424 | 1.00 | 25.10 | O |
| ATOM | 735 | CB | GLU | A | 110 | 28.136 | 5.221 | 8.624 | 1.00 | 24.23 | C |
| ATOM | 736 | N | HIS | A | 111 | 26.035 | 4.974 | 6.201 | 1.00 | 25.65 | N |
| ATOM | 737 | CA | HIS | A | 111 | 25.430 | 4.048 | 5.248 | 1.00 | 26.65 | C |
| ATOM | 738 | C | HIS | A | 111 | 24.667 | 4.718 | 4.101 | 1.00 | 26.96 | C |
| ATOM | 739 | O | HIS | A | 111 | 23.915 | 4.057 | 3.388 | 1.00 | 27.26 | O |
| ATOM | 740 | CB | HIS | A | 111 | 24.566 | 3.015 | 5.979 | 1.00 | 27.06 | C |
| ATOM | 741 | CG | HIS | A | 111 | 25.337 | 2.163 | 6.941 | 1.00 | 27.67 | C |
| ATOM | 742 | ND1 | HIS | A | 111 | 25.385 | 2.424 | 8.294 | 1.00 | 28.34 | N |
| ATOM | 743 | CE1 | HIS | A | 111 | 26.139 | 1.517 | 8.891 | 1.00 | 27.95 | C |
| ATOM | 744 | NE2 | HIS | A | 111 | 26.589 | 0.682 | 7.973 | 1.00 | 28.73 | N |
| ATOM | 745 | CD2 | HIS | A | 111 | 26.105 | 1.065 | 6.744 | 1.00 | 28.20 | C |
| ATOM | 746 | N | LYS | A | 112 | 24.887 | 6.020 | 3.926 | 1.00 | 27.81 | N |
| ATOM | 747 | CA | LYS | A | 112 | 24.351 | 6.804 | 2.810 | 1.00 | 28.57 | C |
| ATOM | 748 | C | LYS | A | 112 | 24.040 | 5.975 | 1.567 | 1.00 | 28.96 | C |
| ATOM | 749 | O | LYS | A | 112 | 22.883 | 5.848 | 1.153 | 1.00 | 29.68 | O |
| ATOM | 750 | CB | LYS | A | 112 | 25.373 | 7.864 | 2.404 | 1.00 | 29.20 | C |
| ATOM | 751 | CG | LYS | A | 112 | 25.185 | 9.227 | 3.019 | 1.00 | 30.74 | C |
| ATOM | 752 | CD | LYS | A | 112 | 25.990 | 10.277 | 2.257 | 1.00 | 31.91 | C |
| ATOM | 753 | CE | LYS | A | 112 | 27.460 | 10.243 | 2.658 | 1.00 | 32.73 | C |
| ATOM | 754 | N | ASP | A | 113 | 25.096 | 5.414 | 0.985 | 1.00 | 28.50 | N |
| ATOM | 755 | CA | ASP | A | 113 | 25.046 | 4.751 | -0.311 | 1.00 | 28.71 | C |
| ATOM | 756 | C | ASP | A | 113 | 24.245 | 3.444 | -0.319 | 1.00 | 28.51 | C |
| ATOM | 757 | O | ASP | A | 113 | 24.078 | 2.817 | -1.370 | 1.00 | 28.24 | O |
| ATOM | 758 | CB | ASP | A | 113 | 26.480 | 4.512 | -0.821 | 1.00 | 28.59 | C |
| ATOM | 759 | N | ASN | A | 114 | 23.746 | 3.047 | 0.848 | 1.00 | 28.67 | N |
| ATOM | 760 | CA | ASN | A | 114 | 23.028 | 1.786 | 1.008 | 1.00 | 28.37 | C |
| ATOM | 761 | C | ASN | A | 114 | 21.589 | 1.949 | 1.495 | 1.00 | 28.14 | C |
| ATOM | 762 | O | ASN | A | 114 | 20.830 | 0.971 | 1.550 | 1.00 | 28.48 | O |
| ATOM | 763 | CB | ASN | A | 114 | 23.796 | 0.878 | 1.969 | 1.00 | 29.15 | C |
| ATOM | 764 | N | ILE | A | 115 | 21.212 | 3.180 | 1.837 | 1.00 | 27.09 | N |
| ATOM | 765 | CA | ILE | A | 115 | 19.898 | 3.441 | 2.420 | 1.00 | 26.21 | C |
| ATOM | 766 | C | ILE | A | 115 | 18.835 | 3.702 | 1.349 | 1.00 | 25.87 | C |
| ATOM | 767 | O | ILE | A | 115 | 18.948 | 4.646 | 0.554 | 1.00 | 26.14 | O |
| ATOM | 768 | CB | ILE | A | 115 | 19.975 | 4.601 | 3.449 | 1.00 | 26.01 | C |
| ATOM | 769 | CG1 | ILE | A | 115 | 20.773 | 4.158 | 4.673 | 1.00 | 25.48 | C |
| ATOM | 770 | CD1 | ILE | A | 115 | 21.239 | 5.287 | 5.543 | 1.00 | 25.59 | C |
| ATOM | 771 | CG2 | ILE | A | 115 | 18.592 | 5.033 | 3.878 | 1.00 | 25.91 | C |
| ATOM | 772 | N | GLY | A | 116 | 17.813 | 2.846 | 1.341 | 1.00 | 24.91 | N |
| ATOM | 773 | CA | GLY | A | 116 | 16.731 | 2.923 | 0.380 | 1.00 | 23.63 | C |
| ATOM | 774 | C | GLY | A | 116 | 15.550 | 3.733 | 0.882 | 1.00 | 23.43 | C |

FIG. 5M

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 775 | O | GLY | A | 116 | 15.502 | 4.152 | 2.050 | 1.00 | 23.30 | O |
| ATOM | 776 | N | SER | A | 117 | 14.582 | 3.943 | -0.004 | 1.00 | 22.42 | N |
| ATOM | 777 | CA | SER | A | 117 | 13.457 | 4.822 | 0.293 | 1.00 | 21.39 | C |
| ATOM | 778 | C | SER | A | 117 | 12.503 | 4.205 | 1.308 | 1.00 | 20.66 | C |
| ATOM | 779 | O | SER | A | 117 | 11.892 | 4.926 | 2.090 | 1.00 | 20.21 | O |
| ATOM | 780 | CB | SER | A | 117 | 12.727 | 5.234 | -0.989 | 1.00 | 21.38 | C |
| ATOM | 781 | OG | SER | A | 117 | 12.203 | 4.108 | -1.669 | 1.00 | 21.36 | O |
| ATOM | 782 | N | GLN | A | 118 | 12.392 | 2.877 | 1.306 | 1.00 | 20.00 | N |
| ATOM | 783 | CA | GLN | A | 118 | 11.538 | 2.190 | 2.273 | 1.00 | 20.08 | C |
| ATOM | 784 | C | GLN | A | 118 | 11.970 | 2.440 | 3.720 | 1.00 | 19.51 | C |
| ATOM | 785 | O | GLN | A | 118 | 11.143 | 2.819 | 4.567 | 1.00 | 19.34 | O |
| ATOM | 786 | CB | GLN | A | 118 | 11.456 | 0.686 | 1.998 | 1.00 | 19.66 | C |
| ATOM | 787 | CG | GLN | A | 118 | 10.421 | -0.030 | 2.876 | 1.00 | 21.00 | C |
| ATOM | 788 | CD | GLN | A | 118 | 8.985 | 0.324 | 2.513 | 1.00 | 22.64 | C |
| ATOM | 789 | OE1 | GLN | A | 118 | 8.403 | -0.281 | 1.615 | 1.00 | 23.31 | O |
| ATOM | 790 | NE2 | GLN | A | 118 | 8.417 | 1.310 | 3.205 | 1.00 | 23.01 | N |
| ATOM | 791 | N | TYR | A | 119 | 13.263 | 2.239 | 3.983 | 1.00 | 19.00 | N |
| ATOM | 792 | CA | TYR | A | 119 | 13.826 | 2.413 | 5.319 | 1.00 | 18.72 | C |
| ATOM | 793 | C | TYR | A | 119 | 13.670 | 3.862 | 5.785 | 1.00 | 18.41 | C |
| ATOM | 794 | O | TYR | A | 119 | 13.241 | 4.109 | 6.917 | 1.00 | 18.22 | O |
| ATOM | 795 | CB | TYR | A | 119 | 15.293 | 1.969 | 5.363 | 1.00 | 18.00 | C |
| ATOM | 796 | CG | TYR | A | 119 | 15.543 | 0.459 | 5.435 | 1.00 | 18.47 | C |
| ATOM | 797 | CD1 | TYR | A | 119 | 16.845 | -0.045 | 5.342 | 1.00 | 18.34 | C |
| ATOM | 798 | CE1 | TYR | A | 119 | 17.110 | -1.412 | 5.406 | 1.00 | 18.42 | C |
| ATOM | 799 | CZ | TYR | A | 119 | 16.071 | -2.307 | 5.565 | 1.00 | 19.18 | C |
| ATOM | 800 | OH | TYR | A | 119 | 16.365 | -3.661 | 5.636 | 1.00 | 18.14 | O |
| ATOM | 801 | CE2 | TYR | A | 119 | 14.751 | -1.841 | 5.664 | 1.00 | 18.93 | C |
| ATOM | 802 | CD2 | TYR | A | 119 | 14.497 | -0.460 | 5.600 | 1.00 | 18.45 | C |
| ATOM | 803 | N | LEU | A | 120 | 13.975 | 4.806 | 4.891 | 1.00 | 18.95 | N |
| ATOM | 804 | CA | LEU | A | 120 | 13.894 | 6.244 | 5.187 | 1.00 | 19.17 | C |
| ATOM | 805 | C | LEU | A | 120 | 12.508 | 6.643 | 5.673 | 1.00 | 18.74 | C |
| ATOM | 806 | O | LEU | A | 120 | 12.363 | 7.299 | 6.707 | 1.00 | 18.45 | O |
| ATOM | 807 | CB | LEU | A | 120 | 14.264 | 7.076 | 3.960 | 1.00 | 19.44 | C |
| ATOM | 808 | CG | LEU | A | 120 | 15.758 | 7.312 | 3.693 | 1.00 | 21.10 | C |
| ATOM | 809 | CD1 | LEU | A | 120 | 15.971 | 7.837 | 2.273 | 1.00 | 20.10 | C |
| ATOM | 810 | CD2 | LEU | A | 120 | 16.409 | 8.248 | 4.728 | 1.00 | 20.90 | C |
| ATOM | 811 | N | LEU | A | 121 | 11.497 | 6.212 | 4.924 | 1.00 | 18.66 | N |
| ATOM | 812 | CA | LEU | A | 121 | 10.109 | 6.510 | 5.227 | 1.00 | 18.36 | C |
| ATOM | 813 | C | LEU | A | 121 | 9.618 | 5.743 | 6.439 | 1.00 | 18.61 | C |
| ATOM | 814 | O | LEU | A | 121 | 8.786 | 6.249 | 7.198 | 1.00 | 19.68 | O |
| ATOM | 815 | CB | LEU | A | 121 | 9.232 | 6.207 | 4.012 | 1.00 | 18.98 | C |
| ATOM | 816 | CG | LEU | A | 121 | 9.392 | 7.129 | 2.793 | 1.00 | 19.19 | C |
| ATOM | 817 | CD1 | LEU | A | 121 | 8.703 | 6.515 | 1.584 | 1.00 | 18.33 | C |
| ATOM | 818 | CD2 | LEU | A | 121 | 8.850 | 8.551 | 3.060 | 1.00 | 18.58 | C |
| ATOM | 819 | N | ASN | A | 122 | 10.120 | 4.520 | 6.622 | 1.00 | 18.38 | N |
| ATOM | 820 | CA | ASN | A | 122 | 9.759 | 3.706 | 7.786 | 1.00 | 17.11 | C |
| ATOM | 821 | C | ASN | A | 122 | 10.309 | 4.315 | 9.065 | 1.00 | 16.63 | C |
| ATOM | 822 | O | ASN | A | 122 | 9.713 | 4.157 | 10.132 | 1.00 | 16.54 | O |
| ATOM | 823 | CB | ASN | A | 122 | 10.263 | 2.262 | 7.653 | 1.00 | 17.07 | C |
| ATOM | 824 | CG | ASN | A | 122 | 9.367 | 1.386 | 6.768 | 1.00 | 17.24 | C |
| ATOM | 825 | OD1 | ASN | A | 122 | 8.336 | 1.819 | 6.253 | 1.00 | 17.42 | O |
| ATOM | 826 | ND2 | ASN | A | 122 | 9.780 | 0.142 | 6.587 | 1.00 | 17.01 | N |
| ATOM | 827 | N | TRP | A | 123 | 11.450 | 4.995 | 8.963 | 1.00 | 15.72 | N |
| ATOM | 828 | CA | TRP | A | 123 | 12.001 | 5.711 | 10.113 | 1.00 | 15.48 | C |
| ATOM | 829 | C | TRP | A | 123 | 11.105 | 6.893 | 10.473 | 1.00 | 15.29 | C |
| ATOM | 830 | O | TRP | A | 123 | 10.834 | 7.121 | 11.644 | 1.00 | 15.63 | O |
| ATOM | 831 | CB | TRP | A | 123 | 13.454 | 6.171 | 9.870 | 1.00 | 15.22 | C |
| ATOM | 832 | CG | TRP | A | 123 | 14.436 | 5.053 | 9.685 | 1.00 | 14.30 | C |
| ATOM | 833 | CD1 | TRP | A | 123 | 14.354 | 3.788 | 10.207 | 1.00 | 14.15 | C |
| ATOM | 834 | NE1 | TRP | A | 123 | 15.441 | 3.041 | 9.810 | 1.00 | 15.26 | N |

FIG. 5N

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 835 | CE2 | TRP | A | 123 | 16.257 | 3.817 | 9.025 | 1.00 | 14.52 | C |
| ATOM | 836 | CD2 | TRP | A | 123 | 15.654 | 5.092 | 8.924 | 1.00 | 13.71 | C |
| ATOM | 837 | CE3 | TRP | A | 123 | 16.304 | 6.080 | 8.167 | 1.00 | 13.55 | C |
| ATOM | 838 | CZ3 | TRP | A | 123 | 17.513 | 5.765 | 7.533 | 1.00 | 12.79 | C |
| ATOM | 839 | CH2 | TRP | A | 123 | 18.084 | 4.489 | 7.656 | 1.00 | 13.28 | C |
| ATOM | 840 | CZ2 | TRP | A | 123 | 17.476 | 3.503 | 8.393 | 1.00 | 14.31 | C |
| ATOM | 841 | N | CYS | A | 124 | 10.634 | 7.625 | 9.460 | 1.00 | 15.14 | N |
| ATOM | 842 | CA | CYS | A | 124 | 9.698 | 8.736 | 9.660 | 1.00 | 15.21 | C |
| ATOM | 843 | C | CYS | A | 124 | 8.424 | 8.311 | 10.374 | 1.00 | 14.82 | C |
| ATOM | 844 | O | CYS | A | 124 | 7.975 | 8.985 | 11.306 | 1.00 | 14.56 | O |
| ATOM | 845 | CB | CYS | A | 124 | 9.313 | 9.371 | 8.324 | 1.00 | 15.93 | C |
| ATOM | 846 | SG | CYS | A | 124 | 10.641 | 10.270 | 7.513 | 1.00 | 16.36 | S |
| ATOM | 847 | N | VAL | A | 125 | 7.838 | 7.203 | 9.919 | 1.00 | 14.31 | N |
| ATOM | 848 | CA | VAL | A | 125 | 6.629 | 6.654 | 10.524 | 1.00 | 13.89 | C |
| ATOM | 849 | C | VAL | A | 125 | 6.894 | 6.286 | 11.980 | 1.00 | 14.21 | C |
| ATOM | 850 | O | VAL | A | 125 | 6.124 | 6.649 | 12.874 | 1.00 | 14.19 | O |
| ATOM | 851 | CB | VAL | A | 125 | 6.120 | 5.403 | 9.729 | 1.00 | 14.52 | C |
| ATOM | 852 | CG1 | VAL | A | 125 | 5.024 | 4.644 | 10.486 | 1.00 | 12.49 | C |
| ATOM | 853 | CG2 | VAL | A | 125 | 5.643 | 5.801 | 8.344 | 1.00 | 13.42 | C |
| ATOM | 854 | N | GLN | A | 126 | 8.003 | 5.586 | 12.211 | 1.00 | 14.40 | N |
| ATOM | 855 | CA | GLN | A | 126 | 8.347 | 5.096 | 13.550 | 1.00 | 14.70 | C |
| ATOM | 856 | C | GLN | A | 126 | 8.545 | 6.203 | 14.576 | 1.00 | 14.00 | C |
| ATOM | 857 | O | GLN | A | 126 | 8.036 | 6.108 | 15.698 | 1.00 | 13.54 | O |
| ATOM | 858 | CB | GLN | A | 126 | 9.578 | 4.195 | 13.490 | 1.00 | 15.10 | C |
| ATOM | 859 | CG | GLN | A | 126 | 9.282 | 2.826 | 12.880 | 1.00 | 17.17 | C |
| ATOM | 860 | CD | GLN | A | 126 | 10.525 | 1.999 | 12.700 | 1.00 | 20.96 | C |
| ATOM | 861 | OE1 | GLN | A | 126 | 11.302 | 1.830 | 13.639 | 1.00 | 22.68 | O |
| ATOM | 862 | NE2 | GLN | A | 126 | 10.728 | 1.486 | 11.492 | 1.00 | 22.88 | N |
| ATOM | 863 | N | ILE | A | 127 | 9.278 | 7.246 | 14.184 | 1.00 | 13.37 | N |
| ATOM | 864 | CA | ILE | A | 127 | 9.502 | 8.412 | 15.042 | 1.00 | 13.63 | C |
| ATOM | 865 | C | ILE | A | 127 | 8.181 | 9.135 | 15.346 | 1.00 | 13.10 | C |
| ATOM | 866 | O | ILE | A | 127 | 7.969 | 9.594 | 16.462 | 1.00 | 13.28 | O |
| ATOM | 867 | CB | ILE | A | 127 | 10.581 | 9.376 | 14.424 | 1.00 | 13.61 | C |
| ATOM | 868 | CG1 | ILE | A | 127 | 11.936 | 8.671 | 14.311 | 1.00 | 12.05 | C |
| ATOM | 869 | CD1 | ILE | A | 127 | 12.841 | 9.240 | 13.224 | 1.00 | 11.70 | C |
| ATOM | 870 | CG2 | ILE | A | 127 | 10.769 | 10.620 | 15.283 | 1.00 | 13.78 | C |
| ATOM | 871 | N | ALA | A | 128 | 7.289 | 9.199 | 14.361 | 1.00 | 13.28 | N |
| ATOM | 872 | CA | ALA | A | 128 | 5.961 | 9.778 | 14.555 | 1.00 | 13.03 | C |
| ATOM | 873 | C | ALA | A | 128 | 5.155 | 8.960 | 15.552 | 1.00 | 13.27 | C |
| ATOM | 874 | O | ALA | A | 128 | 4.450 | 9.517 | 16.391 | 1.00 | 13.14 | O |
| ATOM | 875 | CB | ALA | A | 128 | 5.214 | 9.894 | 13.228 | 1.00 | 12.73 | C |
| ATOM | 876 | N | LYS | A | 129 | 5.267 | 7.637 | 15.454 | 1.00 | 13.85 | N |
| ATOM | 877 | CA | LYS | A | 129 | 4.575 | 6.725 | 16.362 | 1.00 | 14.17 | C |
| ATOM | 878 | C | LYS | A | 129 | 4.990 | 6.930 | 17.819 | 1.00 | 14.33 | C |
| ATOM | 879 | O | LYS | A | 129 | 4.147 | 6.851 | 18.721 | 1.00 | 13.89 | O |
| ATOM | 880 | CB | LYS | A | 129 | 4.805 | 5.273 | 15.947 | 1.00 | 13.58 | C |
| ATOM | 881 | CG | LYS | A | 129 | 3.909 | 4.845 | 14.796 | 1.00 | 15.97 | C |
| ATOM | 882 | CD | LYS | A | 129 | 4.103 | 3.379 | 14.398 | 1.00 | 16.91 | C |
| ATOM | 883 | CE | LYS | A | 129 | 3.195 | 3.037 | 13.222 | 1.00 | 19.68 | C |
| ATOM | 884 | NZ | LYS | A | 129 | 3.293 | 1.603 | 12.810 | 1.00 | 22.45 | N |
| ATOM | 885 | N | GLY | A | 130 | 6.286 | 7.185 | 18.032 | 1.00 | 13.96 | N |
| ATOM | 886 | CA | GLY | A | 130 | 6.839 | 7.334 | 19.360 | 1.00 | 14.09 | C |
| ATOM | 887 | C | GLY | A | 130 | 6.523 | 8.694 | 19.952 | 1.00 | 14.58 | C |
| ATOM | 888 | O | GLY | A | 130 | 6.305 | 8.838 | 21.154 | 1.00 | 14.52 | O |
| ATOM | 889 | N | MET | A | 131 | 6.513 | 9.701 | 19.092 | 1.00 | 14.84 | N |
| ATOM | 890 | CA | MET | A | 131 | 6.190 | 11.053 | 19.502 | 1.00 | 14.50 | C |
| ATOM | 891 | C | MET | A | 131 | 4.703 | 11.145 | 19.830 | 1.00 | 14.37 | C |
| ATOM | 892 | O | MET | A | 131 | 4.324 | 11.734 | 20.845 | 1.00 | 14.31 | O |
| ATOM | 893 | CB | MET | A | 131 | 6.586 | 12.041 | 18.401 | 1.00 | 15.08 | C |
| ATOM | 894 | CG | MET | A | 131 | 8.087 | 12.293 | 18.237 | 1.00 | 14.49 | C |

FIG. 50

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 895 | SD | MET | A | 131 | 9.027 | 12.425 | 19.792 | 1.00 | 17.42 | S |
| ATOM | 896 | CE | MET | A | 131 | 8.633 | 14.034 | 20.326 | 1.00 | 17.35 | C |
| ATOM | 897 | N | ASN | A | 132 | 3.870 | 10.531 | 18.989 | 1.00 | 14.50 | N |
| ATOM | 898 | CA | ASN | A | 132 | 2.442 | 10.400 | 19.264 | 1.00 | 14.90 | C |
| ATOM | 899 | C | ASN | A | 132 | 2.143 | 9.729 | 20.608 | 1.00 | 15.41 | C |
| ATOM | 900 | O | ASN | A | 132 | 1.257 | 10.190 | 21.348 | 1.00 | 15.26 | O |
| ATOM | 901 | CB | ASN | A | 132 | 1.726 | 9.659 | 18.138 | 1.00 | 15.21 | C |
| ATOM | 902 | CG | ASN | A | 132 | 0.207 | 9.659 | 18.303 | 1.00 | 16.33 | C |
| ATOM | 903 | OD1 | ASN | A | 132 | -0.443 | 10.671 | 18.090 | 1.00 | 17.58 | O |
| ATOM | 904 | ND2 | ASN | A | 132 | -0.355 | 8.514 | 18.679 | 1.00 | 16.50 | N |
| ATOM | 905 | N | TYR | A | 133 | 2.873 | 8.653 | 20.922 | 1.00 | 14.99 | N |
| ATOM | 906 | CA | TYR | A | 133 | 2.712 | 7.982 | 22.214 | 1.00 | 15.40 | C |
| ATOM | 907 | C | TYR | A | 133 | 3.041 | 8.947 | 23.351 | 1.00 | 15.44 | C |
| ATOM | 908 | O | TYR | A | 133 | 2.349 | 8.973 | 24.371 | 1.00 | 15.16 | O |
| ATOM | 909 | CB | TYR | A | 133 | 3.590 | 6.728 | 22.319 | 1.00 | 15.46 | C |
| ATOM | 910 | CG | TYR | A | 133 | 3.726 | 6.200 | 23.732 | 1.00 | 15.71 | C |
| ATOM | 911 | CD1 | TYR | A | 133 | 2.803 | 5.288 | 24.248 | 1.00 | 14.82 | C |
| ATOM | 912 | CE1 | TYR | A | 133 | 2.917 | 4.804 | 25.545 | 1.00 | 14.41 | C |
| ATOM | 913 | CZ | TYR | A | 133 | 3.959 | 5.233 | 26.350 | 1.00 | 15.35 | C |
| ATOM | 914 | OH | TYR | A | 133 | 4.063 | 4.755 | 27.643 | 1.00 | 15.78 | O |
| ATOM | 915 | CE2 | TYR | A | 133 | 4.892 | 6.144 | 25.868 | 1.00 | 15.46 | C |
| ATOM | 916 | CD2 | TYR | A | 133 | 4.774 | 6.622 | 24.563 | 1.00 | 16.54 | C |
| ATOM | 917 | N | LEU | A | 134 | 4.106 | 9.729 | 23.163 | 1.00 | 15.72 | N |
| ATOM | 918 | CA | LEU | A | 134 | 4.535 | 10.708 | 24.154 | 1.00 | 15.87 | C |
| ATOM | 919 | C | LEU | A | 134 | 3.459 | 11.773 | 24.326 | 1.00 | 16.01 | C |
| ATOM | 920 | O | LEU | A | 134 | 3.154 | 12.170 | 25.450 | 1.00 | 16.23 | O |
| ATOM | 921 | CB | LEU | A | 134 | 5.867 | 11.333 | 23.742 | 1.00 | 15.78 | C |
| ATOM | 922 | CG | LEU | A | 134 | 7.162 | 10.908 | 24.441 | 1.00 | 16.15 | C |
| ATOM | 923 | CD1 | LEU | A | 134 | 7.075 | 9.522 | 25.075 | 1.00 | 15.74 | C |
| ATOM | 924 | CD2 | LEU | A | 134 | 8.360 | 11.003 | 23.496 | 1.00 | 13.85 | C |
| ATOM | 925 | N | GLU | A | 135 | 2.879 | 12.204 | 23.204 | 1.00 | 16.46 | N |
| ATOM | 926 | CA | GLU | A | 135 | 1.778 | 13.164 | 23.193 | 1.00 | 17.29 | C |
| ATOM | 927 | C | GLU | A | 135 | 0.523 | 12.628 | 23.905 | 1.00 | 17.62 | C |
| ATOM | 928 | O | GLU | A | 135 | -0.066 | 13.334 | 24.726 | 1.00 | 17.96 | O |
| ATOM | 929 | CB | GLU | A | 135 | 1.460 | 13.605 | 21.755 | 1.00 | 17.14 | C |
| ATOM | 930 | CG | GLU | A | 135 | 0.089 | 14.238 | 21.575 | 1.00 | 18.32 | C |
| ATOM | 931 | CD | GLU | A | 135 | 0.024 | 15.261 | 20.457 | 1.00 | 20.06 | C |
| ATOM | 932 | OE1 | GLU | A | 135 | -0.705 | 16.270 | 20.628 | 1.00 | 19.86 | O |
| ATOM | 933 | OE2 | GLU | A | 135 | 0.682 | 15.061 | 19.406 | 1.00 | 21.64 | O |
| ATOM | 934 | N | ASP | A | 136 | 0.127 | 11.390 | 23.600 | 1.00 | 17.99 | N |
| ATOM | 935 | CA | ASP | A | 136 | -1.043 | 10.772 | 24.220 | 1.00 | 18.35 | C |
| ATOM | 936 | C | ASP | A | 136 | -0.874 | 10.707 | 25.733 | 1.00 | 19.10 | C |
| ATOM | 937 | O | ASP | A | 136 | -1.845 | 10.796 | 26.483 | 1.00 | 18.65 | O |
| ATOM | 938 | CB | ASP | A | 136 | -1.257 | 9.358 | 23.698 | 1.00 | 18.04 | C |
| ATOM | 939 | CG | ASP | A | 136 | -1.944 | 9.314 | 22.336 | 1.00 | 18.87 | C |
| ATOM | 940 | OD1 | ASP | A | 136 | -2.681 | 10.265 | 21.956 | 1.00 | 16.22 | O |
| ATOM | 941 | OD2 | ASP | A | 136 | -1.801 | 8.322 | 21.582 | 1.00 | 18.98 | O |
| ATOM | 942 | N | ARG | A | 137 | 0.372 | 10.544 | 26.167 | 1.00 | 19.72 | N |
| ATOM | 943 | CA | ARG | A | 137 | 0.703 | 10.498 | 27.582 | 1.00 | 20.48 | C |
| ATOM | 944 | C | ARG | A | 137 | 0.945 | 11.900 | 28.142 | 1.00 | 20.61 | C |
| ATOM | 945 | O | ARG | A | 137 | 1.317 | 12.045 | 29.301 | 1.00 | 20.07 | O |
| ATOM | 946 | CB | ARG | A | 137 | 1.934 | 9.619 | 27.797 | 1.00 | 21.19 | C |
| ATOM | 947 | CG | ARG | A | 137 | 1.603 | 8.144 | 27.976 | 1.00 | 22.61 | C |
| ATOM | 948 | CD | ARG | A | 137 | 1.636 | 7.689 | 29.416 | 1.00 | 24.32 | C |
| ATOM | 949 | NE | ARG | A | 137 | 2.892 | 6.993 | 29.659 | 1.00 | 26.86 | N |
| ATOM | 950 | CZ | ARG | A | 137 | 3.675 | 7.191 | 30.698 | 1.00 | 26.31 | C |
| ATOM | 951 | NH1 | ARG | A | 137 | 3.350 | 8.063 | 31.638 | 1.00 | 25.50 | N |
| ATOM | 952 | NH2 | ARG | A | 137 | 4.802 | 6.509 | 30.790 | 1.00 | 28.28 | N |
| ATOM | 953 | N | ARG | A | 138 | 0.723 | 12.918 | 27.305 | 1.00 | 20.71 | N |
| ATOM | 954 | CA | ARG | A | 138 | 0.954 | 14.324 | 27.660 | 1.00 | 21.45 | C |

FIG. 5P

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 955 | C | ARG | A | 138 | 2.372 | 14.556 | 28.187 | 1.00 | 21.36 | C |
| ATOM | 956 | O | ARG | A | 138 | 2.590 | 15.297 | 29.145 | 1.00 | 22.23 | O |
| ATOM | 957 | CB | ARG | A | 138 | -0.111 | 14.852 | 28.638 | 1.00 | 21.55 | C |
| ATOM | 958 | N | LEU | A | 139 | 3.326 | 13.905 | 27.536 | 1.00 | 21.31 | N |
| ATOM | 959 | CA | LEU | A | 139 | 4.737 | 14.082 | 27.818 | 1.00 | 20.72 | C |
| ATOM | 960 | C | LEU | A | 139 | 5.388 | 14.796 | 26.642 | 1.00 | 19.91 | C |
| ATOM | 961 | O | LEU | A | 139 | 5.127 | 14.451 | 25.486 | 1.00 | 20.46 | O |
| ATOM | 962 | CB | LEU | A | 139 | 5.391 | 12.723 | 28.042 | 1.00 | 21.21 | C |
| ATOM | 963 | CG | LEU | A | 139 | 4.891 | 11.908 | 29.236 | 1.00 | 22.10 | C |
| ATOM | 964 | CD1 | LEU | A | 139 | 5.500 | 10.508 | 29.198 | 1.00 | 21.82 | C |
| ATOM | 965 | CD2 | LEU | A | 139 | 5.193 | 12.621 | 30.562 | 1.00 | 22.12 | C |
| ATOM | 966 | N | VAL | A | 140 | 6.203 | 15.803 | 26.940 | 1.00 | 18.80 | N |
| ATOM | 967 | CA | VAL | A | 140 | 6.874 | 16.616 | 25.925 | 1.00 | 17.97 | C |
| ATOM | 968 | C | VAL | A | 140 | 8.355 | 16.261 | 25.929 | 1.00 | 18.17 | C |
| ATOM | 969 | O | VAL | A | 140 | 8.998 | 16.315 | 26.979 | 1.00 | 18.14 | O |
| ATOM | 970 | CB | VAL | A | 140 | 6.674 | 18.157 | 26.183 | 1.00 | 18.07 | C |
| ATOM | 971 | CG1 | VAL | A | 140 | 7.520 | 19.010 | 25.212 | 1.00 | 17.71 | C |
| ATOM | 972 | CG2 | VAL | A | 140 | 5.203 | 18.546 | 26.068 | 1.00 | 15.63 | C |
| ATOM | 973 | N | HIS | A | 141 | 8.896 | 15.889 | 24.767 | 1.00 | 17.99 | N |
| ATOM | 974 | CA | HIS | A | 141 | 10.299 | 15.458 | 24.685 | 1.00 | 17.67 | C |
| ATOM | 975 | C | HIS | A | 141 | 11.287 | 16.612 | 24.830 | 1.00 | 18.35 | C |
| ATOM | 976 | O | HIS | A | 141 | 12.211 | 16.529 | 25.645 | 1.00 | 17.90 | O |
| ATOM | 977 | CB | HIS | A | 141 | 10.582 | 14.676 | 23.390 | 1.00 | 16.89 | C |
| ATOM | 978 | CG | HIS | A | 141 | 11.887 | 13.942 | 23.405 | 1.00 | 15.60 | C |
| ATOM | 979 | ND1 | HIS | A | 141 | 13.103 | 14.578 | 23.267 | 1.00 | 14.91 | N |
| ATOM | 980 | CE1 | HIS | A | 141 | 14.075 | 13.684 | 23.331 | 1.00 | 14.34 | C |
| ATOM | 981 | NE2 | HIS | A | 141 | 13.535 | 12.492 | 23.501 | 1.00 | 13.15 | N |
| ATOM | 982 | CD2 | HIS | A | 141 | 12.169 | 12.625 | 23.559 | 1.00 | 14.70 | C |
| ATOM | 983 | N | ARG | A | 142 | 11.100 | 17.653 | 24.010 | 1.00 | 19.05 | N |
| ATOM | 984 | CA | ARG | A | 142 | 11.910 | 18.896 | 24.004 | 1.00 | 20.24 | C |
| ATOM | 985 | C | ARG | A | 142 | 13.244 | 18.846 | 23.253 | 1.00 | 19.86 | C |
| ATOM | 986 | O | ARG | A | 142 | 13.824 | 19.900 | 22.958 | 1.00 | 20.25 | O |
| ATOM | 987 | CB | ARG | A | 142 | 12.174 | 19.438 | 25.416 | 1.00 | 20.56 | C |
| ATOM | 988 | CG | ARG | A | 142 | 10.944 | 19.745 | 26.217 | 1.00 | 24.00 | C |
| ATOM | 989 | CD | ARG | A | 142 | 11.195 | 19.734 | 27.703 | 1.00 | 28.85 | C |
| ATOM | 990 | NE | ARG | A | 142 | 11.586 | 21.058 | 28.172 | 1.00 | 32.64 | N |
| ATOM | 991 | CZ | ARG | A | 142 | 10.759 | 21.916 | 28.759 | 1.00 | 34.42 | C |
| ATOM | 992 | NH1 | ARG | A | 142 | 9.483 | 21.594 | 28.962 | 1.00 | 35.67 | N |
| ATOM | 993 | NH2 | ARG | A | 142 | 11.213 | 23.094 | 29.150 | 1.00 | 35.05 | N |
| ATOM | 994 | N | ASP | A | 143 | 13.745 | 17.649 | 22.965 | 1.00 | 19.33 | N |
| ATOM | 995 | CA | ASP | A | 143 | 15.061 | 17.515 | 22.325 | 1.00 | 19.01 | C |
| ATOM | 996 | C | ASP | A | 143 | 15.095 | 16.435 | 21.228 | 1.00 | 17.92 | C |
| ATOM | 997 | O | ASP | A | 143 | 16.052 | 15.667 | 21.119 | 1.00 | 17.22 | O |
| ATOM | 998 | CB | ASP | A | 143 | 16.154 | 17.288 | 23.387 | 1.00 | 19.42 | C |
| ATOM | 999 | CG | ASP | A | 143 | 17.570 | 17.549 | 22.861 | 1.00 | 21.49 | C |
| ATOM | 1000 | OD1 | ASP | A | 143 | 17.743 | 18.171 | 21.784 | 1.00 | 21.44 | O |
| ATOM | 1001 | OD2 | ASP | A | 143 | 18.588 | 17.150 | 23.475 | 1.00 | 23.75 | O |
| ATOM | 1002 | N | LEU | A | 144 | 14.045 | 16.401 | 20.408 | 1.00 | 16.80 | N |
| ATOM | 1003 | CA | LEU | A | 144 | 14.001 | 15.512 | 19.247 | 1.00 | 15.90 | C |
| ATOM | 1004 | C | LEU | A | 144 | 14.982 | 15.974 | 18.179 | 1.00 | 15.48 | C |
| ATOM | 1005 | O | LEU | A | 144 | 14.974 | 17.150 | 17.794 | 1.00 | 15.10 | O |
| ATOM | 1006 | CB | LEU | A | 144 | 12.581 | 15.438 | 18.659 | 1.00 | 15.84 | C |
| ATOM | 1007 | CG | LEU | A | 144 | 12.357 | 14.438 | 17.512 | 1.00 | 15.36 | C |
| ATOM | 1008 | CD1 | LEU | A | 144 | 12.730 | 13.011 | 17.911 | 1.00 | 13.15 | C |
| ATOM | 1009 | CD2 | LEU | A | 144 | 10.919 | 14.499 | 17.038 | 1.00 | 15.96 | C |
| ATOM | 1010 | N | ALA | A | 145 | 15.820 | 15.038 | 17.719 | 1.00 | 14.73 | N |
| ATOM | 1011 | CA | ALA | A | 145 | 16.845 | 15.275 | 16.693 | 1.00 | 13.65 | C |
| ATOM | 1012 | C | ALA | A | 145 | 17.372 | 13.912 | 16.272 | 1.00 | 13.72 | C |
| ATOM | 1013 | O | ALA | A | 145 | 17.207 | 12.940 | 17.025 | 1.00 | 13.86 | O |
| ATOM | 1014 | CB | ALA | A | 145 | 17.983 | 16.119 | 17.250 | 1.00 | 13.19 | C |

FIG. 5Q

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1015 | N | ALA | A | 146 | 18.020 | 13.826 | 15.105 | 1.00 | 12.64 | N |
| ATOM | 1016 | CA | ALA | A | 146 | 18.538 | 12.538 | 14.628 | 1.00 | 12.88 | C |
| ATOM | 1017 | C | ALA | A | 146 | 19.587 | 11.911 | 15.566 | 1.00 | 13.31 | C |
| ATOM | 1018 | O | ALA | A | 146 | 19.693 | 10.679 | 15.653 | 1.00 | 13.58 | O |
| ATOM | 1019 | CB | ALA | A | 146 | 19.073 | 12.649 | 13.221 | 1.00 | 12.31 | C |
| ATOM | 1020 | N | ARG | A | 147 | 20.335 | 12.756 | 16.280 | 1.00 | 13.66 | N |
| ATOM | 1021 | CA | ARG | A | 147 | 21.287 | 12.297 | 17.297 | 1.00 | 14.09 | C |
| ATOM | 1022 | C | ARG | A | 147 | 20.560 | 11.659 | 18.480 | 1.00 | 14.44 | C |
| ATOM | 1023 | O | ARG | A | 147 | 21.163 | 10.927 | 19.255 | 1.00 | 14.85 | O |
| ATOM | 1024 | CB | ARG | A | 147 | 22.187 | 13.451 | 17.782 | 1.00 | 14.71 | C |
| ATOM | 1025 | CG | ARG | A | 147 | 21.422 | 14.659 | 18.329 | 1.00 | 14.43 | C |
| ATOM | 1026 | CD | ARG | A | 147 | 22.251 | 15.715 | 19.062 | 1.00 | 15.49 | C |
| ATOM | 1027 | NE | ARG | A | 147 | 21.360 | 16.732 | 19.626 | 1.00 | 16.41 | N |
| ATOM | 1028 | CZ | ARG | A | 147 | 20.892 | 17.788 | 18.951 | 1.00 | 18.11 | C |
| ATOM | 1029 | NH1 | ARG | A | 147 | 21.269 | 18.004 | 17.693 | 1.00 | 18.16 | N |
| ATOM | 1030 | NH2 | ARG | A | 147 | 20.061 | 18.643 | 19.537 | 1.00 | 16.89 | N |
| ATOM | 1031 | N | ASN | A | 148 | 19.262 | 11.938 | 18.607 | 1.00 | 14.46 | N |
| ATOM | 1032 | CA | ASN | A | 148 | 18.454 | 11.421 | 19.707 | 1.00 | 14.71 | C |
| ATOM | 1033 | C | ASN | A | 148 | 17.480 | 10.299 | 19.289 | 1.00 | 14.74 | C |
| ATOM | 1034 | O | ASN | A | 148 | 16.562 | 9.931 | 20.034 | 1.00 | 13.85 | O |
| ATOM | 1035 | CB | ASN | A | 148 | 17.732 | 12.576 | 20.416 | 1.00 | 14.71 | C |
| ATOM | 1036 | CG | ASN | A | 148 | 18.652 | 13.346 | 21.353 | 1.00 | 16.18 | C |
| ATOM | 1037 | OD1 | ASN | A | 148 | 19.732 | 12.875 | 21.704 | 1.00 | 19.21 | O |
| ATOM | 1038 | ND2 | ASN | A | 148 | 18.230 | 14.533 | 21.761 | 1.00 | 16.91 | N |
| ATOM | 1039 | N | VAL | A | 149 | 17.694 | 9.762 | 18.090 | 1.00 | 14.34 | N |
| ATOM | 1040 | CA | VAL | A | 149 | 17.011 | 8.553 | 17.658 | 1.00 | 14.49 | C |
| ATOM | 1041 | C | VAL | A | 149 | 18.071 | 7.456 | 17.578 | 1.00 | 14.54 | C |
| ATOM | 1042 | O | VAL | A | 149 | 19.134 | 7.658 | 17.002 | 1.00 | 14.91 | O |
| ATOM | 1043 | CB | VAL | A | 149 | 16.287 | 8.735 | 16.294 | 1.00 | 14.23 | C |
| ATOM | 1044 | CG1 | VAL | A | 149 | 15.564 | 7.459 | 15.882 | 1.00 | 13.72 | C |
| ATOM | 1045 | CG2 | VAL | A | 149 | 15.314 | 9.907 | 16.341 | 1.00 | 13.59 | C |
| ATOM | 1046 | N | LEU | A | 150 | 17.789 | 6.310 | 18.185 | 1.00 | 14.84 | N |
| ATOM | 1047 | CA | LEU | A | 150 | 18.741 | 5.203 | 18.198 | 1.00 | 15.61 | C |
| ATOM | 1048 | C | LEU | A | 150 | 18.242 | 4.053 | 17.337 | 1.00 | 15.54 | C |
| ATOM | 1049 | O | LEU | A | 150 | 17.045 | 3.919 | 17.105 | 1.00 | 16.01 | O |
| ATOM | 1050 | CB | LEU | A | 150 | 19.025 | 4.721 | 19.628 | 1.00 | 14.77 | C |
| ATOM | 1051 | CG | LEU | A | 150 | 19.612 | 5.692 | 20.657 | 1.00 | 16.11 | C |
| ATOM | 1052 | CD1 | LEU | A | 150 | 19.742 | 5.017 | 22.040 | 1.00 | 14.87 | C |
| ATOM | 1053 | CD2 | LEU | A | 150 | 20.949 | 6.306 | 20.210 | 1.00 | 15.56 | C |
| ATOM | 1054 | N | VAL | A | 151 | 19.177 | 3.225 | 16.887 | 1.00 | 16.30 | N |
| ATOM | 1055 | CA | VAL | A | 151 | 18.899 | 2.137 | 15.960 | 1.00 | 16.74 | C |
| ATOM | 1056 | C | VAL | A | 151 | 19.056 | 0.795 | 16.673 | 1.00 | 17.53 | C |
| ATOM | 1057 | O | VAL | A | 151 | 20.166 | 0.388 | 17.030 | 1.00 | 17.31 | O |
| ATOM | 1058 | CB | VAL | A | 151 | 19.849 | 2.194 | 14.724 | 1.00 | 16.51 | C |
| ATOM | 1059 | CG1 | VAL | A | 151 | 19.427 | 1.205 | 13.656 | 1.00 | 15.96 | C |
| ATOM | 1060 | CG2 | VAL | A | 151 | 19.929 | 3.595 | 14.149 | 1.00 | 15.50 | C |
| ATOM | 1061 | N | LYS | A | 152 | 17.931 | 0.121 | 16.885 | 1.00 | 18.49 | N |
| ATOM | 1062 | CA | LYS | A | 152 | 17.926 | -1.217 | 17.470 | 1.00 | 19.20 | C |
| ATOM | 1063 | C | LYS | A | 152 | 18.276 | -2.229 | 16.377 | 1.00 | 19.12 | C |
| ATOM | 1064 | O | LYS | A | 152 | 19.193 | -3.038 | 16.541 | 1.00 | 19.20 | O |
| ATOM | 1065 | CB | LYS | A | 152 | 16.561 | -1.503 | 18.110 | 1.00 | 19.41 | C |
| ATOM | 1066 | CG | LYS | A | 152 | 16.160 | -2.964 | 18.186 | 1.00 | 21.14 | C |
| ATOM | 1067 | CD | LYS | A | 152 | 16.606 | -3.604 | 19.479 | 1.00 | 23.55 | C |
| ATOM | 1068 | CE | LYS | A | 152 | 15.576 | -4.587 | 19.975 | 1.00 | 24.60 | C |
| ATOM | 1069 | NZ | LYS | A | 152 | 14.195 | -4.098 | 19.681 | 1.00 | 26.65 | N |
| ATOM | 1070 | N | THR | A | 153 | 17.518 | -2.179 | 15.281 | 1.00 | 18.93 | N |
| ATOM | 1071 | CA | THR | A | 153 | 17.873 | -2.814 | 14.003 | 1.00 | 19.32 | C |
| ATOM | 1072 | C | THR | A | 153 | 17.679 | -1.748 | 12.922 | 1.00 | 19.14 | C |
| ATOM | 1073 | O | THR | A | 153 | 16.933 | -0.791 | 13.146 | 1.00 | 18.51 | O |
| ATOM | 1074 | CB | THR | A | 153 | 16.963 | -4.012 | 13.681 | 1.00 | 18.49 | C |

FIG. 5R

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1075 | OG1 | THR | A | 153 | 15.668 | -3.529 | 13.306 | 1.00 | 18.93 | O |
| ATOM | 1076 | CG2 | THR | A | 153 | 16.680 | -4.866 | 14.912 | 1.00 | 19.22 | C |
| ATOM | 1077 | N | PRO | A | 154 | 18.307 | -1.905 | 11.754 | 1.00 | 19.47 | N |
| ATOM | 1078 | CA | PRO | A | 154 | 18.166 | -0.912 | 10.674 | 1.00 | 19.95 | C |
| ATOM | 1079 | C | PRO | A | 154 | 16.715 | -0.642 | 10.284 | 1.00 | 20.01 | C |
| ATOM | 1080 | O | PRO | A | 154 | 16.429 | 0.399 | 9.702 | 1.00 | 20.48 | O |
| ATOM | 1081 | CB | PRO | A | 154 | 18.940 | -1.544 | 9.520 | 1.00 | 19.75 | C |
| ATOM | 1082 | CG | PRO | A | 154 | 19.956 | -2.383 | 10.204 | 1.00 | 19.57 | C |
| ATOM | 1083 | CD | PRO | A | 154 | 19.200 | -3.007 | 11.351 | 1.00 | 19.61 | C |
| ATOM | 1084 | N | GLN | A | 155 | 15.811 | -1.550 | 10.633 | 1.00 | 20.52 | N |
| ATOM | 1085 | CA | GLN | A | 155 | 14.391 | -1.348 | 10.359 | 1.00 | 20.99 | C |
| ATOM | 1086 | C | GLN | A | 155 | 13.574 | -0.922 | 11.592 | 1.00 | 20.58 | C |
| ATOM | 1087 | O | GLN | A | 155 | 12.384 | -0.651 | 11.468 | 1.00 | 21.14 | O |
| ATOM | 1088 | CB | GLN | A | 155 | 13.774 | -2.568 | 9.645 | 1.00 | 21.50 | C |
| ATOM | 1089 | CG | GLN | A | 155 | 14.100 | -3.939 | 10.239 | 1.00 | 22.63 | C |
| ATOM | 1090 | CD | GLN | A | 155 | 15.398 | -4.554 | 9.706 | 1.00 | 22.97 | C |
| ATOM | 1091 | OE1 | GLN | A | 155 | 16.340 | -4.754 | 10.465 | 1.00 | 23.72 | O |
| ATOM | 1092 | NE2 | GLN | A | 155 | 15.434 | -4.872 | 8.421 | 1.00 | 22.60 | N |
| ATOM | 1093 | N | HIS | A | 156 | 14.224 | -0.834 | 12.758 | 1.00 | 20.02 | N |
| ATOM | 1094 | CA | HIS | A | 156 | 13.561 | -0.470 | 14.013 | 1.00 | 19.04 | C |
| ATOM | 1095 | C | HIS | A | 156 | 14.307 | 0.609 | 14.816 | 1.00 | 18.95 | C |
| ATOM | 1096 | O | HIS | A | 156 | 15.363 | 0.352 | 15.410 | 1.00 | 18.48 | O |
| ATOM | 1097 | CB | HIS | A | 156 | 13.350 | -1.712 | 14.871 | 1.00 | 19.37 | C |
| ATOM | 1098 | CG | HIS | A | 156 | 12.531 | -1.476 | 16.101 | 1.00 | 19.41 | C |
| ATOM | 1099 | ND1 | HIS | A | 156 | 12.141 | -2.501 | 16.934 | 1.00 | 19.90 | N |
| ATOM | 1100 | CE1 | HIS | A | 156 | 11.434 | -2.011 | 17.935 | 1.00 | 19.60 | C |
| ATOM | 1101 | NE2 | HIS | A | 156 | 11.357 | -0.701 | 17.787 | 1.00 | 20.22 | N |
| ATOM | 1102 | CD2 | HIS | A | 156 | 12.030 | -0.341 | 16.643 | 1.00 | 20.26 | C |
| ATOM | 1103 | N | VAL | A | 157 | 13.734 | 1.814 | 14.839 | 1.00 | 18.44 | N |
| ATOM | 1104 | CA | VAL | A | 157 | 14.306 | 2.934 | 15.586 | 1.00 | 17.60 | C |
| ATOM | 1105 | C | VAL | A | 157 | 13.487 | 3.330 | 16.818 | 1.00 | 17.83 | C |
| ATOM | 1106 | O | VAL | A | 157 | 12.290 | 3.018 | 16.922 | 1.00 | 16.77 | O |
| ATOM | 1107 | CB | VAL | A | 157 | 14.559 | 4.177 | 14.690 | 1.00 | 17.96 | C |
| ATOM | 1108 | CG1 | VAL | A | 157 | 15.529 | 3.850 | 13.556 | 1.00 | 16.46 | C |
| ATOM | 1109 | CG2 | VAL | A | 157 | 13.233 | 4.787 | 14.161 | 1.00 | 16.94 | C |
| ATOM | 1110 | N | LYS | A | 158 | 14.165 | 4.022 | 17.736 | 1.00 | 17.71 | N |
| ATOM | 1111 | CA | LYS | A | 158 | 13.635 | 4.412 | 19.039 | 1.00 | 17.71 | C |
| ATOM | 1112 | C | LYS | A | 158 | 14.125 | 5.810 | 19.406 | 1.00 | 17.50 | C |
| ATOM | 1113 | O | LYS | A | 158 | 15.315 | 6.137 | 19.254 | 1.00 | 16.92 | O |
| ATOM | 1114 | CB | LYS | A | 158 | 14.111 | 3.436 | 20.121 | 1.00 | 18.27 | C |
| ATOM | 1115 | CG | LYS | A | 158 | 13.147 | 2.320 | 20.455 | 1.00 | 19.57 | C |
| ATOM | 1116 | CD | LYS | A | 158 | 13.790 | 0.970 | 20.204 | 1.00 | 21.17 | C |
| ATOM | 1117 | CE | LYS | A | 158 | 13.154 | -0.136 | 21.038 | 1.00 | 21.90 | C |
| ATOM | 1118 | NZ | LYS | A | 158 | 13.278 | 0.051 | 22.513 | 1.00 | 21.84 | N |
| ATOM | 1119 | N | ILE | A | 159 | 13.200 | 6.633 | 19.880 | 1.00 | 17.27 | N |
| ATOM | 1120 | CA | ILE | A | 159 | 13.528 | 7.946 | 20.408 | 1.00 | 17.48 | C |
| ATOM | 1121 | C | ILE | A | 159 | 14.154 | 7.758 | 21.792 | 1.00 | 17.64 | C |
| ATOM | 1122 | O | ILE | A | 159 | 13.612 | 7.050 | 22.651 | 1.00 | 17.31 | O |
| ATOM | 1123 | CB | ILE | A | 159 | 12.250 | 8.845 | 20.468 | 1.00 | 18.03 | C |
| ATOM | 1124 | CG1 | ILE | A | 159 | 11.590 | 8.923 | 19.089 | 1.00 | 17.36 | C |
| ATOM | 1125 | CD1 | ILE | A | 159 | 10.074 | 9.055 | 19.146 | 1.00 | 18.32 | C |
| ATOM | 1126 | CG2 | ILE | A | 159 | 12.576 | 10.256 | 20.952 | 1.00 | 16.87 | C |
| ATOM | 1127 | N | THR | A | 160 | 15.309 | 8.379 | 21.994 | 1.00 | 18.18 | N |
| ATOM | 1128 | CA | THR | A | 160 | 16.008 | 8.283 | 23.263 | 1.00 | 19.24 | C |
| ATOM | 1129 | C | THR | A | 160 | 16.080 | 9.622 | 23.978 | 1.00 | 20.13 | C |
| ATOM | 1130 | O | THR | A | 160 | 15.748 | 10.665 | 23.405 | 1.00 | 19.57 | O |
| ATOM | 1131 | CB | THR | A | 160 | 17.419 | 7.697 | 23.067 | 1.00 | 19.37 | C |
| ATOM | 1132 | OG1 | THR | A | 160 | 17.915 | 7.229 | 24.327 | 1.00 | 20.74 | O |
| ATOM | 1133 | CG2 | THR | A | 160 | 18.425 | 8.781 | 22.681 | 1.00 | 18.67 | C |
| ATOM | 1134 | N | ASP | A | 161 | 16.518 | 9.561 | 25.235 | 1.00 | 21.59 | N |

FIG. 5S

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1135 | CA | ASP | A | 161 | 16.777 | 10.730 | 26.075 | 1.00 | 23.05 | C |
| ATOM | 1136 | C | ASP | A | 161 | 15.535 | 11.523 | 26.457 | 1.00 | 23.74 | C |
| ATOM | 1137 | O | ASP | A | 161 | 15.641 | 12.702 | 26.774 | 1.00 | 23.97 | O |
| ATOM | 1138 | CB | ASP | A | 161 | 17.813 | 11.658 | 25.436 | 1.00 | 23.33 | C |
| ATOM | 1139 | CG | ASP | A | 161 | 19.199 | 11.053 | 25.410 | 1.00 | 24.80 | C |
| ATOM | 1140 | OD1 | ASP | A | 161 | 19.364 | 9.908 | 25.893 | 1.00 | 25.43 | O |
| ATOM | 1141 | OD2 | ASP | A | 161 | 20.185 | 11.654 | 24.923 | 1.00 | 26.18 | O |
| ATOM | 1142 | N | PHE | A | 162 | 14.364 | 10.895 | 26.435 | 1.00 | 24.61 | N |
| ATOM | 1143 | CA | PHE | A | 162 | 13.202 | 11.552 | 27.008 | 1.00 | 26.22 | C |
| ATOM | 1144 | C | PHE | A | 162 | 13.470 | 11.808 | 28.495 | 1.00 | 27.55 | C |
| ATOM | 1145 | O | PHE | A | 162 | 13.898 | 10.899 | 29.220 | 1.00 | 27.82 | O |
| ATOM | 1146 | CB | PHE | A | 162 | 11.924 | 10.733 | 26.858 | 1.00 | 25.70 | C |
| ATOM | 1147 | CG | PHE | A | 162 | 10.799 | 11.272 | 27.677 | 1.00 | 26.29 | C |
| ATOM | 1148 | CD1 | PHE | A | 162 | 10.144 | 12.440 | 27.288 | 1.00 | 26.33 | C |
| ATOM | 1149 | CE1 | PHE | A | 162 | 9.126 | 12.973 | 28.053 | 1.00 | 26.57 | C |
| ATOM | 1150 | CZ | PHE | A | 162 | 8.756 | 12.339 | 29.240 | 1.00 | 27.93 | C |
| ATOM | 1151 | CE2 | PHE | A | 162 | 9.414 | 11.179 | 29.644 | 1.00 | 27.04 | C |
| ATOM | 1152 | CD2 | PHE | A | 162 | 10.431 | 10.655 | 28.865 | 1.00 | 26.37 | C |
| ATOM | 1153 | N | GLY | A | 163 | 13.232 | 13.044 | 28.933 | 1.00 | 28.52 | N |
| ATOM | 1154 | CA | GLY | A | 163 | 13.381 | 13.404 | 30.332 | 1.00 | 29.88 | C |
| ATOM | 1155 | C | GLY | A | 163 | 14.786 | 13.822 | 30.747 | 1.00 | 31.02 | C |
| ATOM | 1156 | O | GLY | A | 163 | 14.985 | 14.270 | 31.879 | 1.00 | 31.42 | O |
| ATOM | 1157 | N | LEU | A | 164 | 15.754 | 13.699 | 29.841 | 1.00 | 31.58 | N |
| ATOM | 1158 | CA | LEU | A | 164 | 17.139 | 14.054 | 30.144 | 1.00 | 32.81 | C |
| ATOM | 1159 | C | LEU | A | 164 | 17.390 | 15.572 | 30.253 | 1.00 | 33.77 | C |
| ATOM | 1160 | O | LEU | A | 164 | 18.513 | 16.042 | 30.050 | 1.00 | 34.62 | O |
| ATOM | 1161 | CB | LEU | A | 164 | 18.094 | 13.420 | 29.121 | 1.00 | 32.62 | C |
| ATOM | 1162 | CG | LEU | A | 164 | 19.010 | 12.275 | 29.568 | 1.00 | 33.16 | C |
| ATOM | 1163 | CD1 | LEU | A | 164 | 20.130 | 12.049 | 28.556 | 1.00 | 32.69 | C |
| ATOM | 1164 | CD2 | LEU | A | 164 | 19.594 | 12.488 | 30.964 | 1.00 | 32.89 | C |
| ATOM | 1165 | N | ALA | A | 165 | 16.341 | 16.337 | 30.549 | 1.00 | 34.73 | N |
| ATOM | 1166 | CA | ALA | A | 165 | 16.480 | 17.750 | 30.899 | 1.00 | 34.93 | C |
| ATOM | 1167 | C | ALA | A | 165 | 16.058 | 17.965 | 32.347 | 1.00 | 34.94 | C |
| ATOM | 1168 | O | ALA | A | 165 | 14.934 | 17.632 | 32.730 | 1.00 | 35.00 | O |
| ATOM | 1169 | CB | ALA | A | 165 | 15.649 | 18.626 | 29.964 | 1.00 | 34.93 | C |
| ATOM | 1170 | N | VAL | A | 182 | 20.301 | 25.244 | 23.844 | 1.00 | 34.28 | N |
| ATOM | 1171 | CA | VAL | A | 182 | 21.537 | 24.924 | 23.126 | 1.00 | 34.05 | C |
| ATOM | 1172 | C | VAL | A | 182 | 21.286 | 24.339 | 21.719 | 1.00 | 33.33 | C |
| ATOM | 1173 | O | VAL | A | 182 | 22.023 | 24.664 | 20.779 | 1.00 | 33.82 | O |
| ATOM | 1174 | CB | VAL | A | 182 | 22.482 | 24.006 | 23.964 | 1.00 | 34.30 | C |
| ATOM | 1175 | CG1 | VAL | A | 182 | 23.807 | 23.759 | 23.235 | 1.00 | 34.94 | C |
| ATOM | 1176 | CG2 | VAL | A | 182 | 22.763 | 24.622 | 25.327 | 1.00 | 34.84 | C |
| ATOM | 1177 | N | PRO | A | 183 | 20.272 | 23.480 | 21.566 | 1.00 | 32.37 | N |
| ATOM | 1178 | CA | PRO | A | 183 | 19.931 | 22.921 | 20.253 | 1.00 | 31.01 | C |
| ATOM | 1179 | C | PRO | A | 183 | 18.912 | 23.790 | 19.503 | 1.00 | 29.64 | C |
| ATOM | 1180 | O | PRO | A | 183 | 17.915 | 23.292 | 18.963 | 1.00 | 28.78 | O |
| ATOM | 1181 | CB | PRO | A | 183 | 19.328 | 21.570 | 20.619 | 1.00 | 31.41 | C |
| ATOM | 1182 | CG | PRO | A | 183 | 18.673 | 21.801 | 21.951 | 1.00 | 32.01 | C |
| ATOM | 1183 | CD | PRO | A | 183 | 19.394 | 22.934 | 22.620 | 1.00 | 32.31 | C |
| ATOM | 1184 | N | ILE | A | 184 | 19.208 | 25.085 | 19.459 | 1.00 | 27.89 | N |
| ATOM | 1185 | CA | ILE | A | 184 | 18.358 | 26.104 | 18.855 | 1.00 | 26.36 | C |
| ATOM | 1186 | C | ILE | A | 184 | 17.994 | 25.794 | 17.397 | 1.00 | 25.09 | C |
| ATOM | 1187 | O | ILE | A | 184 | 16.944 | 26.217 | 16.909 | 1.00 | 24.14 | O |
| ATOM | 1188 | CB | ILE | A | 184 | 19.042 | 27.508 | 19.028 | 1.00 | 26.74 | C |
| ATOM | 1189 | CG1 | ILE | A | 184 | 18.573 | 28.161 | 20.335 | 1.00 | 27.39 | C |
| ATOM | 1190 | CD1 | ILE | A | 184 | 19.678 | 28.809 | 21.158 | 1.00 | 28.47 | C |
| ATOM | 1191 | CG2 | ILE | A | 184 | 18.802 | 28.430 | 17.828 | 1.00 | 25.89 | C |
| ATOM | 1192 | N | LYS | A | 185 | 18.847 | 25.031 | 16.718 | 1.00 | 23.81 | N |
| ATOM | 1193 | CA | LYS | A | 185 | 18.609 | 24.697 | 15.316 | 1.00 | 22.96 | C |
| ATOM | 1194 | C | LYS | A | 185 | 17.531 | 23.626 | 15.104 | 1.00 | 22.85 | C |

FIG. 5T

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1195 | O | LYS | A | 185 | 17.097 | 23.404 | 13.973 | 1.00 | 22.66 | O |
| ATOM | 1196 | CB | LYS | A | 185 | 19.919 | 24.338 | 14.609 | 1.00 | 22.77 | C |
| ATOM | 1197 | CG | LYS | A | 185 | 20.730 | 25.562 | 14.203 | 1.00 | 21.39 | C |
| ATOM | 1198 | CD | LYS | A | 185 | 22.182 | 25.206 | 13.920 | 1.00 | 20.35 | C |
| ATOM | 1199 | CE | LYS | A | 185 | 23.029 | 26.453 | 13.674 | 1.00 | 20.37 | C |
| ATOM | 1200 | NZ | LYS | A | 185 | 23.928 | 26.311 | 12.485 | 1.00 | 19.49 | N |
| ATOM | 1201 | N | TRP | A | 186 | 17.104 | 22.982 | 16.194 | 1.00 | 22.62 | N |
| ATOM | 1202 | CA | TRP | A | 186 | 16.002 | 22.010 | 16.185 | 1.00 | 22.33 | C |
| ATOM | 1203 | C | TRP | A | 186 | 14.740 | 22.555 | 16.866 | 1.00 | 22.97 | C |
| ATOM | 1204 | O | TRP | A | 186 | 13.693 | 21.899 | 16.876 | 1.00 | 23.08 | O |
| ATOM | 1205 | CB | TRP | A | 186 | 16.432 | 20.698 | 16.871 | 1.00 | 21.32 | C |
| ATOM | 1206 | CG | TRP | A | 186 | 17.310 | 19.853 | 16.016 | 1.00 | 19.73 | C |
| ATOM | 1207 | CD1 | TRP | A | 186 | 16.942 | 18.750 | 15.303 | 1.00 | 19.03 | C |
| ATOM | 1208 | NE1 | TRP | A | 186 | 18.020 | 18.249 | 14.611 | 1.00 | 18.84 | N |
| ATOM | 1209 | CE2 | TRP | A | 186 | 19.120 | 19.028 | 14.872 | 1.00 | 18.48 | C |
| ATOM | 1210 | CD2 | TRP | A | 186 | 18.708 | 20.055 | 15.749 | 1.00 | 18.88 | C |
| ATOM | 1211 | CE3 | TRP | A | 186 | 19.661 | 20.997 | 16.174 | 1.00 | 18.93 | C |
| ATOM | 1212 | CZ3 | TRP | A | 186 | 20.974 | 20.887 | 15.712 | 1.00 | 18.06 | C |
| ATOM | 1213 | CH2 | TRP | A | 186 | 21.348 | 19.854 | 14.837 | 1.00 | 17.52 | C |
| ATOM | 1214 | CZ2 | TRP | A | 186 | 20.438 | 18.918 | 14.405 | 1.00 | 18.20 | C |
| ATOM | 1215 | N | MET | A | 187 | 14.841 | 23.755 | 17.435 | 1.00 | 23.39 | N |
| ATOM | 1216 | CA | MET | A | 187 | 13.775 | 24.307 | 18.273 | 1.00 | 23.57 | C |
| ATOM | 1217 | C | MET | A | 187 | 12.724 | 25.075 | 17.483 | 1.00 | 23.43 | C |
| ATOM | 1218 | O | MET | A | 187 | 13.046 | 25.757 | 16.503 | 1.00 | 22.77 | O |
| ATOM | 1219 | CB | MET | A | 187 | 14.366 | 25.233 | 19.340 | 1.00 | 24.11 | C |
| ATOM | 1220 | CG | MET | A | 187 | 15.173 | 24.546 | 20.430 | 1.00 | 25.91 | C |
| ATOM | 1221 | SD | MET | A | 187 | 15.856 | 25.764 | 21.577 | 1.00 | 27.80 | S |
| ATOM | 1222 | CE | MET | A | 187 | 16.354 | 24.734 | 22.912 | 1.00 | 29.88 | C |
| ATOM | 1223 | N | ALA | A | 188 | 11.471 | 24.969 | 17.931 | 1.00 | 23.51 | N |
| ATOM | 1224 | CA | ALA | A | 188 | 10.369 | 25.768 | 17.397 | 1.00 | 23.42 | C |
| ATOM | 1225 | C | ALA | A | 188 | 10.548 | 27.224 | 17.782 | 1.00 | 23.86 | C |
| ATOM | 1226 | O | ALA | A | 188 | 11.052 | 27.529 | 18.867 | 1.00 | 23.74 | O |
| ATOM | 1227 | CB | ALA | A | 188 | 9.049 | 25.269 | 17.923 | 1.00 | 23.97 | C |
| ATOM | 1228 | N | LEU | A | 189 | 10.122 | 28.120 | 16.894 | 1.00 | 23.46 | N |
| ATOM | 1229 | CA | LEU | A | 189 | 10.252 | 29.556 | 17.116 | 1.00 | 23.33 | C |
| ATOM | 1230 | C | LEU | A | 189 | 9.754 | 30.012 | 18.503 | 1.00 | 22.77 | C |
| ATOM | 1231 | O | LEU | A | 189 | 10.386 | 30.845 | 19.145 | 1.00 | 22.70 | O |
| ATOM | 1232 | CB | LEU | A | 189 | 9.556 | 30.339 | 15.992 | 1.00 | 23.03 | C |
| ATOM | 1233 | CG | LEU | A | 189 | 9.810 | 31.850 | 16.017 | 1.00 | 24.06 | C |
| ATOM | 1234 | CD1 | LEU | A | 189 | 11.118 | 32.210 | 15.327 | 1.00 | 24.21 | C |
| ATOM | 1235 | CD2 | LEU | A | 189 | 8.640 | 32.618 | 15.412 | 1.00 | 24.58 | C |
| ATOM | 1236 | N | GLU | A | 190 | 8.628 | 29.464 | 18.956 | 1.00 | 22.39 | N |
| ATOM | 1237 | CA | GLU | A | 190 | 8.091 | 29.809 | 20.269 | 1.00 | 22.22 | C |
| ATOM | 1238 | C | GLU | A | 190 | 8.980 | 29.286 | 21.399 | 1.00 | 22.30 | C |
| ATOM | 1239 | O | GLU | A | 190 | 8.964 | 29.826 | 22.512 | 1.00 | 22.15 | O |
| ATOM | 1240 | CB | GLU | A | 190 | 6.655 | 29.299 | 20.424 | 1.00 | 22.28 | C |
| ATOM | 1241 | CG | GLU | A | 190 | 6.526 | 27.784 | 20.499 | 1.00 | 22.56 | C |
| ATOM | 1242 | CD | GLU | A | 190 | 6.208 | 27.132 | 19.168 | 1.00 | 21.94 | C |
| ATOM | 1243 | OE1 | GLU | A | 190 | 5.625 | 26.035 | 19.195 | 1.00 | 23.30 | O |
| ATOM | 1244 | OE2 | GLU | A | 190 | 6.543 | 27.692 | 18.103 | 1.00 | 21.29 | O |
| ATOM | 1245 | N | SER | A | 191 | 9.761 | 28.246 | 21.104 | 1.00 | 22.37 | N |
| ATOM | 1246 | CA | SER | A | 191 | 10.684 | 27.667 | 22.083 | 1.00 | 22.95 | C |
| ATOM | 1247 | C | SER | A | 191 | 11.905 | 28.549 | 22.255 | 1.00 | 23.25 | C |
| ATOM | 1248 | O | SER | A | 191 | 12.376 | 28.747 | 23.373 | 1.00 | 23.31 | O |
| ATOM | 1249 | CB | SER | A | 191 | 11.096 | 26.243 | 21.702 | 1.00 | 22.56 | C |
| ATOM | 1250 | OG | SER | A | 191 | 9.974 | 25.376 | 21.685 | 1.00 | 22.32 | O |
| ATOM | 1251 | N | ILE | A | 192 | 12.400 | 29.101 | 21.155 | 1.00 | 23.97 | N |
| ATOM | 1252 | CA | ILE | A | 192 | 13.561 | 29.980 | 21.230 | 1.00 | 25.49 | C |
| ATOM | 1253 | C | ILE | A | 192 | 13.206 | 31.314 | 21.882 | 1.00 | 25.96 | C |
| ATOM | 1254 | O | ILE | A | 192 | 13.903 | 31.756 | 22.796 | 1.00 | 26.30 | O |

FIG. 5U

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1255 | CB | ILE | A | 192 | 14.223 | 30.217 | 19.850 | 1.00 | 25.50 | C |
| ATOM | 1256 | CG1 | ILE | A | 192 | 14.327 | 28.916 | 19.040 | 1.00 | 25.40 | C |
| ATOM | 1257 | CD1 | ILE | A | 192 | 14.569 | 29.122 | 17.549 | 1.00 | 25.46 | C |
| ATOM | 1258 | CG2 | ILE | A | 192 | 15.599 | 30.835 | 20.048 | 1.00 | 26.28 | C |
| ATOM | 1259 | N | LEU | A | 193 | 12.120 | 31.934 | 21.418 | 1.00 | 26.25 | N |
| ATOM | 1260 | CA | LEU | A | 193 | 11.747 | 33.278 | 21.863 | 1.00 | 26.69 | C |
| ATOM | 1261 | C | LEU | A | 193 | 11.138 | 33.323 | 23.260 | 1.00 | 26.63 | C |
| ATOM | 1262 | O | LEU | A | 193 | 11.355 | 34.288 | 23.986 | 1.00 | 27.00 | O |
| ATOM | 1263 | CB | LEU | A | 193 | 10.779 | 33.952 | 20.875 | 1.00 | 26.51 | C |
| ATOM | 1264 | CG | LEU | A | 193 | 11.204 | 34.213 | 19.431 | 1.00 | 27.25 | C |
| ATOM | 1265 | CD1 | LEU | A | 193 | 9.986 | 34.570 | 18.592 | 1.00 | 27.23 | C |
| ATOM | 1266 | CD2 | LEU | A | 193 | 12.269 | 35.301 | 19.333 | 1.00 | 27.77 | C |
| ATOM | 1267 | N | HIS | A | 194 | 10.370 | 32.296 | 23.624 | 1.00 | 26.80 | N |
| ATOM | 1268 | CA | HIS | A | 194 | 9.576 | 32.324 | 24.854 | 1.00 | 26.71 | C |
| ATOM | 1269 | C | HIS | A | 194 | 9.811 | 31.151 | 25.784 | 1.00 | 26.65 | C |
| ATOM | 1270 | O | HIS | A | 194 | 9.300 | 31.143 | 26.899 | 1.00 | 26.84 | O |
| ATOM | 1271 | CB | HIS | A | 194 | 8.080 | 32.403 | 24.534 | 1.00 | 27.00 | C |
| ATOM | 1272 | CG | HIS | A | 194 | 7.724 | 33.456 | 23.528 | 1.00 | 27.89 | C |
| ATOM | 1273 | ND1 | HIS | A | 194 | 8.074 | 34.781 | 23.678 | 1.00 | 28.32 | N |
| ATOM | 1274 | CE1 | HIS | A | 194 | 7.630 | 35.472 | 22.644 | 1.00 | 28.99 | C |
| ATOM | 1275 | NE2 | HIS | A | 194 | 7.000 | 34.643 | 21.830 | 1.00 | 29.74 | N |
| ATOM | 1276 | CD2 | HIS | A | 194 | 7.043 | 33.377 | 22.361 | 1.00 | 28.04 | C |
| ATOM | 1277 | N | ARG | A | 195 | 10.570 | 30.156 | 25.325 | 1.00 | 26.92 | N |
| ATOM | 1278 | CA | ARG | A | 195 | 10.780 | 28.912 | 26.082 | 1.00 | 26.59 | C |
| ATOM | 1279 | C | ARG | A | 195 | 9.465 | 28.151 | 26.370 | 1.00 | 26.41 | C |
| ATOM | 1280 | O | ARG | A | 195 | 9.324 | 27.488 | 27.402 | 1.00 | 26.41 | O |
| ATOM | 1281 | CB | ARG | A | 195 | 11.582 | 29.167 | 27.369 | 1.00 | 26.71 | C |
| ATOM | 1282 | CG | ARG | A | 195 | 12.960 | 29.777 | 27.136 | 1.00 | 26.74 | C |
| ATOM | 1283 | CD | ARG | A | 195 | 14.101 | 28.786 | 27.220 | 1.00 | 26.21 | C |
| ATOM | 1284 | N | ILE | A | 196 | 8.516 | 28.263 | 25.443 | 1.00 | 25.89 | N |
| ATOM | 1285 | CA | ILE | A | 196 | 7.310 | 27.439 | 25.441 | 1.00 | 25.99 | C |
| ATOM | 1286 | C | ILE | A | 196 | 7.605 | 26.110 | 24.723 | 1.00 | 25.37 | C |
| ATOM | 1287 | O | ILE | A | 196 | 8.162 | 26.098 | 23.619 | 1.00 | 25.06 | O |
| ATOM | 1288 | CB | ILE | A | 196 | 6.130 | 28.195 | 24.758 | 1.00 | 26.18 | C |
| ATOM | 1289 | CG1 | ILE | A | 196 | 5.750 | 29.443 | 25.562 | 1.00 | 26.92 | C |
| ATOM | 1290 | CD1 | ILE | A | 196 | 5.022 | 30.515 | 24.750 | 1.00 | 27.60 | C |
| ATOM | 1291 | CG2 | ILE | A | 196 | 4.912 | 27.288 | 24.597 | 1.00 | 26.16 | C |
| ATOM | 1292 | N | TYR | A | 197 | 7.244 | 25.004 | 25.372 | 1.00 | 24.61 | N |
| ATOM | 1293 | CA | TYR | A | 197 | 7.393 | 23.667 | 24.812 | 1.00 | 24.00 | C |
| ATOM | 1294 | C | TYR | A | 197 | 6.072 | 22.926 | 24.894 | 1.00 | 23.38 | C |
| ATOM | 1295 | O | TYR | A | 197 | 5.534 | 22.721 | 25.972 | 1.00 | 23.52 | O |
| ATOM | 1296 | CB | TYR | A | 197 | 8.453 | 22.866 | 25.563 | 1.00 | 24.16 | C |
| ATOM | 1297 | CG | TYR | A | 197 | 9.860 | 23.378 | 25.400 | 1.00 | 24.86 | C |
| ATOM | 1298 | CD1 | TYR | A | 197 | 10.683 | 22.891 | 24.391 | 1.00 | 24.84 | C |
| ATOM | 1299 | CE1 | TYR | A | 197 | 11.980 | 23.354 | 24.239 | 1.00 | 24.86 | C |
| ATOM | 1300 | CZ | TYR | A | 197 | 12.465 | 24.311 | 25.102 | 1.00 | 25.63 | C |
| ATOM | 1301 | OH | TYR | A | 197 | 13.749 | 24.762 | 24.951 | 1.00 | 27.70 | O |
| ATOM | 1302 | CE2 | TYR | A | 197 | 11.674 | 24.814 | 26.119 | 1.00 | 25.54 | C |
| ATOM | 1303 | CD2 | TYR | A | 197 | 10.377 | 24.344 | 26.266 | 1.00 | 25.42 | C |
| ATOM | 1304 | N | THR | A | 198 | 5.551 | 22.536 | 23.739 | 1.00 | 22.68 | N |
| ATOM | 1305 | CA | THR | A | 198 | 4.330 | 21.748 | 23.661 | 1.00 | 21.60 | C |
| ATOM | 1306 | C | THR | A | 198 | 4.578 | 20.581 | 22.712 | 1.00 | 21.30 | C |
| ATOM | 1307 | O | THR | A | 198 | 5.687 | 20.424 | 22.190 | 1.00 | 20.65 | O |
| ATOM | 1308 | CB | THR | A | 198 | 3.183 | 22.600 | 23.103 | 1.00 | 21.35 | C |
| ATOM | 1309 | OG1 | THR | A | 198 | 3.516 | 22.976 | 21.764 | 1.00 | 20.86 | O |
| ATOM | 1310 | CG2 | THR | A | 198 | 3.059 | 23.934 | 23.844 | 1.00 | 20.48 | C |
| ATOM | 1311 | N | HIS | A | 199 | 3.544 | 19.778 | 22.468 | 1.00 | 20.37 | N |
| ATOM | 1312 | CA | HIS | A | 199 | 3.650 | 18.715 | 21.473 | 1.00 | 20.11 | C |
| ATOM | 1313 | C | HIS | A | 199 | 3.859 | 19.272 | 20.059 | 1.00 | 19.90 | C |
| ATOM | 1314 | O | HIS | A | 199 | 4.593 | 18.679 | 19.266 | 1.00 | 20.32 | O |

FIG. 5V

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1315 | CB | HIS | A | 199 | 2.433 | 17.793 | 21.522 | 1.00 | 19.71 | C |
| ATOM | 1316 | CG | HIS | A | 199 | 2.009 | 17.440 | 22.909 | 1.00 | 18.90 | C |
| ATOM | 1317 | ND1 | HIS | A | 199 | 2.810 | 16.726 | 23.770 | 1.00 | 18.63 | N |
| ATOM | 1318 | CE1 | HIS | A | 199 | 2.182 | 16.569 | 24.922 | 1.00 | 19.12 | C |
| ATOM | 1319 | NE2 | HIS | A | 199 | 1.006 | 17.170 | 24.842 | 1.00 | 17.97 | N |
| ATOM | 1320 | CD2 | HIS | A | 199 | 0.875 | 17.726 | 23.596 | 1.00 | 18.15 | C |
| ATOM | 1321 | N | GLN | A | 200 | 3.225 | 20.411 | 19.767 | 1.00 | 19.30 | N |
| ATOM | 1322 | CA | GLN | A | 200 | 3.398 | 21.125 | 18.496 | 1.00 | 18.44 | C |
| ATOM | 1323 | C | GLN | A | 200 | 4.818 | 21.653 | 18.323 | 1.00 | 18.49 | C |
| ATOM | 1324 | O | GLN | A | 200 | 5.323 | 21.756 | 17.203 | 1.00 | 18.42 | O |
| ATOM | 1325 | CB | GLN | A | 200 | 2.384 | 22.270 | 18.373 | 1.00 | 17.83 | C |
| ATOM | 1326 | CG | GLN | A | 200 | 0.929 | 21.809 | 18.182 | 1.00 | 16.67 | C |
| ATOM | 1327 | CD | GLN | A | 200 | 0.814 | 20.578 | 17.302 | 1.00 | 17.53 | C |
| ATOM | 1328 | OE1 | GLN | A | 200 | 0.836 | 19.449 | 17.798 | 1.00 | 18.58 | O |
| ATOM | 1329 | NE2 | GLN | A | 200 | 0.704 | 20.788 | 15.998 | 1.00 | 17.73 | N |
| ATOM | 1330 | N | SER | A | 201 | 5.451 | 21.985 | 19.443 | 1.00 | 18.47 | N |
| ATOM | 1331 | CA | SER | A | 201 | 6.865 | 22.338 | 19.471 | 1.00 | 19.01 | C |
| ATOM | 1332 | C | SER | A | 201 | 7.721 | 21.131 | 19.083 | 1.00 | 18.77 | C |
| ATOM | 1333 | O | SER | A | 201 | 8.684 | 21.263 | 18.321 | 1.00 | 19.46 | O |
| ATOM | 1334 | CB | SER | A | 201 | 7.250 | 22.835 | 20.859 | 1.00 | 19.02 | C |
| ATOM | 1335 | OG | SER | A | 201 | 8.541 | 23.382 | 20.837 | 1.00 | 21.15 | O |
| ATOM | 1336 | N | ASP | A | 202 | 7.358 | 19.958 | 19.600 | 1.00 | 18.15 | N |
| ATOM | 1337 | CA | ASP | A | 202 | 7.995 | 18.707 | 19.199 | 1.00 | 17.70 | C |
| ATOM | 1338 | C | ASP | A | 202 | 7.790 | 18.416 | 17.702 | 1.00 | 17.27 | C |
| ATOM | 1339 | O | ASP | A | 202 | 8.660 | 17.821 | 17.062 | 1.00 | 16.39 | O |
| ATOM | 1340 | CB | ASP | A | 202 | 7.491 | 17.536 | 20.060 | 1.00 | 17.82 | C |
| ATOM | 1341 | CG | ASP | A | 202 | 8.248 | 17.401 | 21.395 | 1.00 | 18.25 | C |
| ATOM | 1342 | OD1 | ASP | A | 202 | 7.815 | 16.578 | 22.240 | 1.00 | 19.15 | O |
| ATOM | 1343 | OD2 | ASP | A | 202 | 9.275 | 18.055 | 21.693 | 1.00 | 16.73 | O |
| ATOM | 1344 | N | VAL | A | 203 | 6.651 | 18.846 | 17.147 | 1.00 | 16.84 | N |
| ATOM | 1345 | CA | VAL | A | 203 | 6.355 | 18.615 | 15.729 | 1.00 | 17.10 | C |
| ATOM | 1346 | C | VAL | A | 203 | 7.367 | 19.329 | 14.828 | 1.00 | 17.03 | C |
| ATOM | 1347 | O | VAL | A | 203 | 7.834 | 18.760 | 13.833 | 1.00 | 17.52 | O |
| ATOM | 1348 | CB | VAL | A | 203 | 4.898 | 18.996 | 15.355 | 1.00 | 17.35 | C |
| ATOM | 1349 | CG1 | VAL | A | 203 | 4.711 | 19.069 | 13.818 | 1.00 | 17.32 | C |
| ATOM | 1350 | CG2 | VAL | A | 203 | 3.928 | 18.002 | 15.953 | 1.00 | 16.31 | C |
| ATOM | 1351 | N | TRP | A | 204 | 7.710 | 20.560 | 15.206 | 1.00 | 16.10 | N |
| ATOM | 1352 | CA | TRP | A | 204 | 8.753 | 21.336 | 14.557 | 1.00 | 15.91 | C |
| ATOM | 1353 | C | TRP | A | 204 | 10.102 | 20.608 | 14.569 | 1.00 | 15.34 | C |
| ATOM | 1354 | O | TRP | A | 204 | 10.788 | 20.536 | 13.545 | 1.00 | 14.63 | O |
| ATOM | 1355 | CB | TRP | A | 204 | 8.899 | 22.705 | 15.248 | 1.00 | 16.48 | C |
| ATOM | 1356 | CG | TRP | A | 204 | 9.950 | 23.584 | 14.629 | 1.00 | 17.32 | C |
| ATOM | 1357 | CD1 | TRP | A | 204 | 11.291 | 23.318 | 14.510 | 1.00 | 18.24 | C |
| ATOM | 1358 | NE1 | TRP | A | 204 | 11.929 | 24.357 | 13.876 | 1.00 | 17.48 | N |
| ATOM | 1359 | CE2 | TRP | A | 204 | 11.005 | 25.327 | 13.584 | 1.00 | 19.12 | C |
| ATOM | 1360 | CD2 | TRP | A | 204 | 9.749 | 24.869 | 14.042 | 1.00 | 18.39 | C |
| ATOM | 1361 | CE3 | TRP | A | 204 | 8.633 | 25.699 | 13.871 | 1.00 | 17.73 | C |
| ATOM | 1362 | CZ3 | TRP | A | 204 | 8.799 | 26.918 | 13.254 | 1.00 | 17.80 | C |
| ATOM | 1363 | CH2 | TRP | A | 204 | 10.055 | 27.340 | 12.801 | 1.00 | 18.87 | C |
| ATOM | 1364 | CZ2 | TRP | A | 204 | 11.167 | 26.566 | 12.953 | 1.00 | 19.46 | C |
| ATOM | 1365 | N | SER | A | 205 | 10.482 | 20.084 | 15.731 | 1.00 | 15.10 | N |
| ATOM | 1366 | CA | SER | A | 205 | 11.735 | 19.338 | 15.863 | 1.00 | 15.25 | C |
| ATOM | 1367 | C | SER | A | 205 | 11.733 | 18.081 | 14.991 | 1.00 | 14.79 | C |
| ATOM | 1368 | O | SER | A | 205 | 12.764 | 17.709 | 14.411 | 1.00 | 14.59 | O |
| ATOM | 1369 | CB | SER | A | 205 | 12.000 | 18.990 | 17.323 | 1.00 | 15.02 | C |
| ATOM | 1370 | OG | SER | A | 205 | 12.167 | 20.181 | 18.070 | 1.00 | 16.99 | O |
| ATOM | 1371 | N | TYR | A | 206 | 10.561 | 17.453 | 14.891 | 1.00 | 14.26 | N |
| ATOM | 1372 | CA | TYR | A | 206 | 10.366 | 16.298 | 14.025 | 1.00 | 13.63 | C |
| ATOM | 1373 | C | TYR | A | 206 | 10.655 | 16.661 | 12.566 | 1.00 | 13.14 | C |
| ATOM | 1374 | O | TYR | A | 206 | 11.369 | 15.924 | 11.874 | 1.00 | 13.08 | O |

FIG. 5W

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1375 | CB | TYR | A | 206 | 8.957 | 15.725 | 14.210 | 1.00 | 13.55 | C |
| ATOM | 1376 | CG | TYR | A | 206 | 8.588 | 14.665 | 13.214 | 1.00 | 13.29 | C |
| ATOM | 1377 | CD1 | TYR | A | 206 | 7.982 | 14.999 | 11.993 | 1.00 | 12.45 | C |
| ATOM | 1378 | CE1 | TYR | A | 206 | 7.651 | 14.014 | 11.072 | 1.00 | 14.04 | C |
| ATOM | 1379 | CZ | TYR | A | 206 | 7.920 | 12.674 | 11.378 | 1.00 | 13.69 | C |
| ATOM | 1380 | OH | TYR | A | 206 | 7.608 | 11.678 | 10.492 | 1.00 | 14.65 | O |
| ATOM | 1381 | CE2 | TYR | A | 206 | 8.516 | 12.329 | 12.573 | 1.00 | 14.49 | C |
| ATOM | 1382 | CD2 | TYR | A | 206 | 8.848 | 13.321 | 13.486 | 1.00 | 13.52 | C |
| ATOM | 1383 | N | GLY | A | 207 | 10.123 | 17.799 | 12.112 | 1.00 | 12.72 | N |
| ATOM | 1384 | CA | GLY | A | 207 | 10.437 | 18.342 | 10.795 | 1.00 | 12.45 | C |
| ATOM | 1385 | C | GLY | A | 207 | 11.934 | 18.458 | 10.495 | 1.00 | 13.29 | C |
| ATOM | 1386 | O | GLY | A | 207 | 12.395 | 18.056 | 9.422 | 1.00 | 13.01 | O |
| ATOM | 1387 | N | VAL | A | 208 | 12.699 | 19.001 | 11.441 | 1.00 | 13.39 | N |
| ATOM | 1388 | CA | VAL | A | 208 | 14.147 | 19.117 | 11.276 | 1.00 | 13.82 | C |
| ATOM | 1389 | C | VAL | A | 208 | 14.801 | 17.727 | 11.229 | 1.00 | 14.23 | C |
| ATOM | 1390 | O | VAL | A | 208 | 15.635 | 17.451 | 10.360 | 1.00 | 14.47 | O |
| ATOM | 1391 | CB | VAL | A | 208 | 14.790 | 20.011 | 12.373 | 1.00 | 13.67 | C |
| ATOM | 1392 | CG1 | VAL | A | 208 | 16.292 | 20.150 | 12.144 | 1.00 | 13.84 | C |
| ATOM | 1393 | CG2 | VAL | A | 208 | 14.128 | 21.388 | 12.397 | 1.00 | 12.06 | C |
| ATOM | 1394 | N | THR | A | 209 | 14.398 | 16.853 | 12.148 | 1.00 | 14.37 | N |
| ATOM | 1395 | CA | THR | A | 209 | 14.874 | 15.471 | 12.172 | 1.00 | 15.20 | C |
| ATOM | 1396 | C | THR | A | 209 | 14.654 | 14.774 | 10.824 | 1.00 | 15.26 | C |
| ATOM | 1397 | O | THR | A | 209 | 15.571 | 14.137 | 10.291 | 1.00 | 15.59 | O |
| ATOM | 1398 | CB | THR | A | 209 | 14.184 | 14.690 | 13.300 | 1.00 | 14.65 | C |
| ATOM | 1399 | OG1 | THR | A | 209 | 14.427 | 15.358 | 14.542 | 1.00 | 16.24 | O |
| ATOM | 1400 | CG2 | THR | A | 209 | 14.838 | 13.342 | 13.496 | 1.00 | 14.51 | C |
| ATOM | 1401 | N | VAL | A | 210 | 13.446 | 14.915 | 10.277 | 1.00 | 15.58 | N |
| ATOM | 1402 | CA | VAL | A | 210 | 13.112 | 14.346 | 8.973 | 1.00 | 15.63 | C |
| ATOM | 1403 | C | VAL | A | 210 | 14.022 | 14.933 | 7.898 | 1.00 | 15.81 | C |
| ATOM | 1404 | O | VAL | A | 210 | 14.568 | 14.196 | 7.073 | 1.00 | 16.62 | O |
| ATOM | 1405 | CB | VAL | A | 210 | 11.600 | 14.494 | 8.642 | 1.00 | 16.20 | C |
| ATOM | 1406 | CG1 | VAL | A | 210 | 11.318 | 14.258 | 7.159 | 1.00 | 15.96 | C |
| ATOM | 1407 | CG2 | VAL | A | 210 | 10.773 | 13.530 | 9.495 | 1.00 | 14.14 | C |
| ATOM | 1408 | N | TRP | A | 211 | 14.238 | 16.243 | 7.951 | 1.00 | 15.66 | N |
| ATOM | 1409 | CA | TRP | A | 211 | 15.185 | 16.902 | 7.045 | 1.00 | 15.68 | C |
| ATOM | 1410 | C | TRP | A | 211 | 16.596 | 16.293 | 7.128 | 1.00 | 15.43 | C |
| ATOM | 1411 | O | TRP | A | 211 | 17.213 | 16.045 | 6.090 | 1.00 | 14.91 | O |
| ATOM | 1412 | CB | TRP | A | 211 | 15.230 | 18.422 | 7.292 | 1.00 | 14.80 | C |
| ATOM | 1413 | CG | TRP | A | 211 | 16.078 | 19.158 | 6.320 | 1.00 | 14.08 | C |
| ATOM | 1414 | CD1 | TRP | A | 211 | 15.693 | 19.656 | 5.108 | 1.00 | 13.94 | C |
| ATOM | 1415 | NE1 | TRP | A | 211 | 16.754 | 20.281 | 4.492 | 1.00 | 15.12 | N |
| ATOM | 1416 | CE2 | TRP | A | 211 | 17.859 | 20.187 | 5.295 | 1.00 | 15.19 | C |
| ATOM | 1417 | CD2 | TRP | A | 211 | 17.470 | 19.486 | 6.463 | 1.00 | 15.80 | C |
| ATOM | 1418 | CE3 | TRP | A | 211 | 18.436 | 19.253 | 7.458 | 1.00 | 15.56 | C |
| ATOM | 1419 | CZ3 | TRP | A | 211 | 19.739 | 19.726 | 7.259 | 1.00 | 15.37 | C |
| ATOM | 1420 | CH2 | TRP | A | 211 | 20.085 | 20.426 | 6.093 | 1.00 | 15.50 | C |
| ATOM | 1421 | CH2 | TRP | A | 211 | 19.165 | 20.660 | 5.097 | 1.00 | 16.49 | C |
| ATOM | 1422 | N | GLU | A | 212 | 17.089 | 16.063 | 8.352 | 1.00 | 15.91 | N |
| ATOM | 1423 | CA | GLU | A | 212 | 18.391 | 15.402 | 8.592 | 1.00 | 16.30 | C |
| ATOM | 1424 | C | GLU | A | 212 | 18.495 | 14.048 | 7.917 | 1.00 | 16.81 | C |
| ATOM | 1425 | O | GLU | A | 212 | 19.518 | 13.729 | 7.322 | 1.00 | 17.85 | O |
| ATOM | 1426 | CB | GLU | A | 212 | 18.656 | 15.191 | 10.087 | 1.00 | 16.54 | C |
| ATOM | 1427 | CG | GLU | A | 212 | 18.997 | 16.435 | 10.886 | 1.00 | 16.04 | C |
| ATOM | 1428 | CD | GLU | A | 212 | 19.317 | 16.104 | 12.334 | 1.00 | 16.27 | C |
| ATOM | 1429 | OE1 | GLU | A | 212 | 20.504 | 15.909 | 12.641 | 1.00 | 16.31 | O |
| ATOM | 1430 | OE2 | GLU | A | 212 | 18.381 | 16.039 | 13.168 | 1.00 | 16.78 | O |
| ATOM | 1431 | N | LEU | A | 213 | 17.444 | 13.241 | 8.030 | 1.00 | 17.14 | N |
| ATOM | 1432 | CA | LEU | A | 213 | 17.421 | 11.922 | 7.396 | 1.00 | 17.73 | C |
| ATOM | 1433 | C | LEU | A | 213 | 17.379 | 12.010 | 5.877 | 1.00 | 18.34 | C |
| ATOM | 1434 | O | LEU | A | 213 | 18.054 | 11.235 | 5.195 | 1.00 | 18.78 | O |

FIG. 5X

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1435 | CB | LEU | A | 213 | 16.228 | 11.093 | 7.888 | 1.00 | 17.19 | C |
| ATOM | 1436 | CG | LEU | A | 213 | 16.002 | 10.959 | 9.393 | 1.00 | 17.49 | C |
| ATOM | 1437 | CD1 | LEU | A | 213 | 14.740 | 10.111 | 9.696 | 1.00 | 15.99 | C |
| ATOM | 1438 | CD2 | LEU | A | 213 | 17.262 | 10.385 | 10.065 | 1.00 | 17.13 | C |
| ATOM | 1439 | N | MET | A | 214 | 16.576 | 12.944 | 5.359 | 1.00 | 18.90 | N |
| ATOM | 1440 | CA | MET | A | 214 | 16.388 | 13.109 | 3.917 | 1.00 | 19.52 | C |
| ATOM | 1441 | C | MET | A | 214 | 17.655 | 13.597 | 3.198 | 1.00 | 19.26 | C |
| ATOM | 1442 | O | MET | A | 214 | 17.820 | 13.352 | 2.007 | 1.00 | 19.42 | O |
| ATOM | 1443 | CB | MET | A | 214 | 15.214 | 14.048 | 3.615 | 1.00 | 19.99 | C |
| ATOM | 1444 | CG | MET | A | 214 | 13.822 | 13.488 | 3.928 | 1.00 | 21.85 | C |
| ATOM | 1445 | SD | MET | A | 214 | 13.590 | 11.766 | 3.421 | 1.00 | 25.97 | S |
| ATOM | 1446 | CE | MET | A | 214 | 11.901 | 11.510 | 3.898 | 1.00 | 25.02 | C |
| ATOM | 1447 | N | THR | A | 215 | 18.527 | 14.292 | 3.925 | 1.00 | 18.67 | N |
| ATOM | 1448 | CA | THR | A | 215 | 19.812 | 14.749 | 3.401 | 1.00 | 18.65 | C |
| ATOM | 1449 | C | THR | A | 215 | 20.957 | 13.818 | 3.805 | 1.00 | 19.03 | C |
| ATOM | 1450 | O | THR | A | 215 | 22.121 | 14.155 | 3.599 | 1.00 | 19.86 | O |
| ATOM | 1451 | CB | THR | A | 215 | 20.149 | 16.156 | 3.926 | 1.00 | 18.53 | C |
| ATOM | 1452 | OG1 | THR | A | 215 | 20.177 | 16.134 | 5.364 | 1.00 | 19.23 | O |
| ATOM | 1453 | CG2 | THR | A | 215 | 19.060 | 17.174 | 3.569 | 1.00 | 17.20 | C |
| ATOM | 1454 | N | PHE | A | 216 | 20.630 | 12.671 | 4.406 | 1.00 | 18.91 | N |
| ATOM | 1455 | CA | PHE | A | 216 | 21.627 | 11.707 | 4.892 | 1.00 | 18.62 | C |
| ATOM | 1456 | C | PHE | A | 216 | 22.591 | 12.302 | 5.921 | 1.00 | 18.49 | C |
| ATOM | 1457 | O | PHE | A | 216 | 23.773 | 11.938 | 5.968 | 1.00 | 18.09 | O |
| ATOM | 1458 | CB | PHE | A | 216 | 22.400 | 11.063 | 3.730 | 1.00 | 18.90 | C |
| ATOM | 1459 | CG | PHE | A | 216 | 21.525 | 10.372 | 2.723 | 1.00 | 19.02 | C |
| ATOM | 1460 | CD1 | PHE | A | 216 | 21.113 | 9.060 | 2.925 | 1.00 | 19.29 | C |
| ATOM | 1461 | CE1 | PHE | A | 216 | 20.306 | 8.419 | 2.001 | 1.00 | 19.46 | C |
| ATOM | 1462 | CZ | PHE | A | 216 | 19.900 | 9.094 | 0.848 | 1.00 | 19.99 | C |
| ATOM | 1463 | CE2 | PHE | A | 216 | 20.300 | 10.407 | 0.637 | 1.00 | 19.88 | C |
| ATOM | 1464 | CD2 | PHE | A | 216 | 21.114 | 11.036 | 1.570 | 1.00 | 19.88 | C |
| ATOM | 1465 | N | GLY | A | 217 | 22.079 | 13.230 | 6.731 | 1.00 | 18.54 | N |
| ATOM | 1466 | CA | GLY | A | 217 | 22.787 | 13.715 | 7.902 | 1.00 | 18.62 | C |
| ATOM | 1467 | C | GLY | A | 217 | 23.525 | 15.031 | 7.759 | 1.00 | 19.01 | C |
| ATOM | 1468 | O | GLY | A | 217 | 24.528 | 15.250 | 8.441 | 1.00 | 19.29 | O |
| ATOM | 1469 | N | SER | A | 218 | 23.035 | 15.897 | 6.873 | 1.00 | 19.27 | N |
| ATOM | 1470 | CA | SER | A | 218 | 23.532 | 17.259 | 6.755 | 1.00 | 19.49 | C |
| ATOM | 1471 | C | SER | A | 218 | 23.151 | 18.031 | 8.008 | 1.00 | 20.23 | C |
| ATOM | 1472 | O | SER | A | 218 | 22.185 | 17.677 | 8.705 | 1.00 | 19.99 | O |
| ATOM | 1473 | CB | SER | A | 218 | 22.954 | 17.947 | 5.520 | 1.00 | 19.54 | C |
| ATOM | 1474 | OG | SER | A | 218 | 23.303 | 17.248 | 4.335 | 1.00 | 20.51 | O |
| ATOM | 1475 | N | LYS | A | 219 | 23.920 | 19.078 | 8.293 | 1.00 | 20.46 | N |
| ATOM | 1476 | CA | LYS | A | 219 | 23.733 | 19.870 | 9.493 | 1.00 | 21.27 | C |
| ATOM | 1477 | C | LYS | A | 219 | 22.820 | 21.039 | 9.185 | 1.00 | 21.76 | C |
| ATOM | 1478 | O | LYS | A | 219 | 23.096 | 21.822 | 8.274 | 1.00 | 22.17 | O |
| ATOM | 1479 | CB | LYS | A | 219 | 25.077 | 20.373 | 10.012 | 1.00 | 21.65 | C |
| ATOM | 1480 | CG | LYS | A | 219 | 26.084 | 19.274 | 10.319 | 1.00 | 22.85 | C |
| ATOM | 1481 | CD | LYS | A | 219 | 27.035 | 19.710 | 11.427 | 1.00 | 25.41 | C |
| ATOM | 1482 | CE | LYS | A | 219 | 28.454 | 19.776 | 10.919 | 1.00 | 26.27 | C |
| ATOM | 1483 | NZ | LYS | A | 219 | 29.083 | 18.421 | 11.009 | 1.00 | 28.06 | N |
| ATOM | 1484 | N | PRO | A | 220 | 21.735 | 21.159 | 9.946 | 1.00 | 22.25 | N |
| ATOM | 1485 | CA | PRO | A | 220 | 20.718 | 22.182 | 9.694 | 1.00 | 22.20 | C |
| ATOM | 1486 | C | PRO | A | 220 | 21.304 | 23.584 | 9.813 | 1.00 | 22.73 | C |
| ATOM | 1487 | O | PRO | A | 220 | 21.984 | 23.868 | 10.794 | 1.00 | 22.13 | O |
| ATOM | 1488 | CB | PRO | A | 220 | 19.698 | 21.941 | 10.808 | 1.00 | 22.46 | C |
| ATOM | 1489 | CG | PRO | A | 220 | 19.934 | 20.546 | 11.250 | 1.00 | 22.59 | C |
| ATOM | 1490 | CD | PRO | A | 220 | 21.413 | 20.332 | 11.126 | 1.00 | 22.16 | C |
| ATOM | 1491 | N | TYR | A | 221 | 21.043 | 24.433 | 8.817 | 1.00 | 23.20 | N |
| ATOM | 1492 | CA | TYR | A | 221 | 21.544 | 25.811 | 8.789 | 1.00 | 23.78 | C |
| ATOM | 1493 | C | TYR | A | 221 | 23.060 | 25.894 | 9.010 | 1.00 | 24.48 | C |
| ATOM | 1494 | O | TYR | A | 221 | 23.537 | 26.744 | 9.759 | 1.00 | 24.27 | O |

FIG. 5Y

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1495 | CB | TYR | A | 221 | 20.808 | 26.691 | 9.815 | 1.00 | 23.69 | C |
| ATOM | 1496 | CG | TYR | A | 221 | 19.322 | 26.416 | 9.985 | 1.00 | 23.37 | C |
| ATOM | 1497 | CD1 | TYR | A | 221 | 18.375 | 27.068 | 9.197 | 1.00 | 22.54 | C |
| ATOM | 1498 | CE1 | TYR | A | 221 | 17.011 | 26.833 | 9.365 | 1.00 | 22.37 | C |
| ATOM | 1499 | CZ | TYR | A | 221 | 16.586 | 25.939 | 10.332 | 1.00 | 22.50 | C |
| ATOM | 1500 | OH | TYR | A | 221 | 15.246 | 25.698 | 10.502 | 1.00 | 23.84 | O |
| ATOM | 1501 | CE2 | TYR | A | 221 | 17.501 | 25.275 | 11.128 | 1.00 | 22.72 | C |
| ATOM | 1502 | CD2 | TYR | A | 221 | 18.864 | 25.526 | 10.962 | 1.00 | 23.51 | C |
| ATOM | 1503 | N | ASP | A | 222 | 23.799 | 24.983 | 8.380 | 1.00 | 25.44 | N |
| ATOM | 1504 | CA | ASP | A | 222 | 25.260 | 24.994 | 8.396 | 1.00 | 26.85 | C |
| ATOM | 1505 | C | ASP | A | 222 | 25.785 | 26.354 | 7.931 | 1.00 | 27.42 | C |
| ATOM | 1506 | O | ASP | A | 222 | 25.450 | 26.801 | 6.836 | 1.00 | 27.17 | O |
| ATOM | 1507 | CB | ASP | A | 222 | 25.791 | 23.887 | 7.475 | 1.00 | 27.21 | C |
| ATOM | 1508 | CG | ASP | A | 222 | 27.180 | 23.390 | 7.870 | 1.00 | 28.40 | C |
| ATOM | 1509 | OD1 | ASP | A | 222 | 27.587 | 23.591 | 9.032 | 1.00 | 28.08 | O |
| ATOM | 1510 | OD2 | ASP | A | 222 | 27.929 | 22.771 | 7.077 | 1.00 | 29.38 | O |
| ATOM | 1511 | N | GLY | A | 223 | 26.584 | 27.012 | 8.772 | 1.00 | 28.11 | N |
| ATOM | 1512 | CA | GLY | A | 223 | 27.174 | 28.298 | 8.429 | 1.00 | 28.87 | C |
| ATOM | 1513 | C | GLY | A | 223 | 26.514 | 29.498 | 9.088 | 1.00 | 29.68 | C |
| ATOM | 1514 | O | GLY | A | 223 | 27.079 | 30.589 | 9.109 | 1.00 | 30.14 | O |
| ATOM | 1515 | N | ILE | A | 224 | 25.318 | 29.301 | 9.631 | 1.00 | 29.85 | N |
| ATOM | 1516 | CA | ILE | A | 224 | 24.608 | 30.369 | 10.316 | 1.00 | 30.14 | C |
| ATOM | 1517 | C | ILE | A | 224 | 24.776 | 30.225 | 11.828 | 1.00 | 30.76 | C |
| ATOM | 1518 | O | ILE | A | 224 | 24.560 | 29.142 | 12.375 | 1.00 | 30.59 | O |
| ATOM | 1519 | CB | ILE | A | 224 | 23.121 | 30.366 | 9.919 | 1.00 | 30.03 | C |
| ATOM | 1520 | CG1 | ILE | A | 224 | 22.990 | 30.407 | 8.396 | 1.00 | 29.96 | C |
| ATOM | 1521 | CD1 | ILE | A | 224 | 21.940 | 29.488 | 7.860 | 1.00 | 30.12 | C |
| ATOM | 1522 | CG2 | ILE | A | 224 | 22.371 | 31.541 | 10.556 | 1.00 | 28.97 | C |
| ATOM | 1523 | N | PRO | A | 225 | 25.174 | 31.311 | 12.498 | 1.00 | 31.26 | N |
| ATOM | 1524 | CA | PRO | A | 225 | 25.301 | 31.308 | 13.956 | 1.00 | 31.31 | C |
| ATOM | 1525 | C | PRO | A | 225 | 23.954 | 30.999 | 14.600 | 1.00 | 31.43 | C |
| ATOM | 1526 | O | PRO | A | 225 | 22.914 | 31.427 | 14.089 | 1.00 | 31.28 | O |
| ATOM | 1527 | CB | PRO | A | 225 | 25.732 | 32.749 | 14.271 | 1.00 | 31.36 | C |
| ATOM | 1528 | CG | PRO | A | 225 | 26.346 | 33.247 | 13.016 | 1.00 | 31.12 | C |
| ATOM | 1529 | CD | PRO | A | 225 | 25.534 | 32.626 | 11.924 | 1.00 | 31.41 | C |
| ATOM | 1530 | N | ALA | A | 226 | 23.978 | 30.246 | 15.694 | 1.00 | 31.44 | N |
| ATOM | 1531 | CA | ALA | A | 226 | 22.773 | 29.953 | 16.454 | 1.00 | 32.22 | C |
| ATOM | 1532 | C | ALA | A | 226 | 21.982 | 31.231 | 16.778 | 1.00 | 32.62 | C |
| ATOM | 1533 | O | ALA | A | 226 | 20.746 | 31.218 | 16.796 | 1.00 | 32.15 | O |
| ATOM | 1534 | CB | ALA | A | 226 | 23.124 | 29.197 | 17.731 | 1.00 | 32.17 | C |
| ATOM | 1535 | N | SER | A | 227 | 22.709 | 32.330 | 17.001 | 1.00 | 32.90 | N |
| ATOM | 1536 | CA | SER | A | 227 | 22.118 | 33.608 | 17.404 | 1.00 | 33.47 | C |
| ATOM | 1537 | C | SER | A | 227 | 21.211 | 34.246 | 16.351 | 1.00 | 33.52 | C |
| ATOM | 1538 | O | SER | A | 227 | 20.327 | 35.037 | 16.691 | 1.00 | 33.90 | O |
| ATOM | 1539 | CB | SER | A | 227 | 23.218 | 34.600 | 17.793 | 1.00 | 33.94 | C |
| ATOM | 1540 | OG | SER | A | 227 | 23.896 | 35.093 | 16.644 | 1.00 | 35.00 | O |
| ATOM | 1541 | N | GLU | A | 228 | 21.438 | 33.906 | 15.083 | 1.00 | 33.28 | N |
| ATOM | 1542 | CA | GLU | A | 228 | 20.717 | 34.510 | 13.969 | 1.00 | 33.05 | C |
| ATOM | 1543 | C | GLU | A | 228 | 19.559 | 33.634 | 13.472 | 1.00 | 33.32 | C |
| ATOM | 1544 | O | GLU | A | 228 | 18.856 | 33.990 | 12.520 | 1.00 | 32.92 | O |
| ATOM | 1545 | CB | GLU | A | 228 | 21.691 | 34.804 | 12.825 | 1.00 | 33.17 | C |
| ATOM | 1546 | N | ILE | A | 229 | 19.355 | 32.495 | 14.131 | 1.00 | 33.41 | N |
| ATOM | 1547 | CA | ILE | A | 229 | 18.378 | 31.510 | 13.674 | 1.00 | 33.24 | C |
| ATOM | 1548 | C | ILE | A | 229 | 16.953 | 32.045 | 13.808 | 1.00 | 33.41 | C |
| ATOM | 1549 | O | ILE | A | 229 | 16.162 | 31.983 | 12.858 | 1.00 | 33.36 | O |
| ATOM | 1550 | CB | ILE | A | 229 | 18.577 | 30.149 | 14.409 | 1.00 | 32.76 | C |
| ATOM | 1551 | CG1 | ILE | A | 229 | 19.919 | 29.510 | 14.020 | 1.00 | 32.35 | C |
| ATOM | 1552 | CD1 | ILE | A | 229 | 20.036 | 29.085 | 12.545 | 1.00 | 31.27 | C |
| ATOM | 1553 | CG2 | ILE | A | 229 | 17.421 | 29.189 | 14.132 | 1.00 | 32.57 | C |
| ATOM | 1554 | N | SER | A | 230 | 16.646 | 32.590 | 14.981 | 1.00 | 33.39 | N |

FIG. 5Z

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1555 | CA | SER | A | 230 | 15.353 | 33.210 | 15.239 | 1.00 | 33.74 | C |
| ATOM | 1556 | C | SER | A | 230 | 14.995 | 34.265 | 14.181 | 1.00 | 33.34 | C |
| ATOM | 1557 | O | SER | A | 230 | 13.848 | 34.326 | 13.711 | 1.00 | 33.30 | O |
| ATOM | 1558 | CB | SER | A | 230 | 15.340 | 33.828 | 16.635 | 1.00 | 33.54 | C |
| ATOM | 1559 | OG | SER | A | 230 | 14.191 | 34.630 | 16.803 | 1.00 | 35.77 | O |
| ATOM | 1560 | N | SER | A | 231 | 15.984 | 35.073 | 13.807 | 1.00 | 32.79 | N |
| ATOM | 1561 | CA | SER | A | 231 | 15.806 | 36.133 | 12.816 | 1.00 | 32.99 | C |
| ATOM | 1562 | C | SER | A | 231 | 15.484 | 35.593 | 11.411 | 1.00 | 32.68 | C |
| ATOM | 1563 | O | SER | A | 231 | 14.515 | 36.043 | 10.785 | 1.00 | 32.87 | O |
| ATOM | 1564 | CB | SER | A | 231 | 17.022 | 37.078 | 12.814 | 1.00 | 33.23 | C |
| ATOM | 1565 | OG | SER | A | 231 | 17.413 | 37.472 | 11.507 | 1.00 | 34.42 | O |
| ATOM | 1566 | N | ILE | A | 232 | 16.262 | 34.625 | 10.924 | 1.00 | 31.98 | N |
| ATOM | 1567 | CA | ILE | A | 232 | 15.977 | 34.042 | 9.608 | 1.00 | 32.09 | C |
| ATOM | 1568 | C | ILE | A | 232 | 14.602 | 33.354 | 9.545 | 1.00 | 31.80 | C |
| ATOM | 1569 | O | ILE | A | 232 | 13.931 | 33.399 | 8.510 | 1.00 | 31.72 | O |
| ATOM | 1570 | CB | ILE | A | 232 | 17.141 | 33.128 | 9.064 | 1.00 | 32.38 | C |
| ATOM | 1571 | CG1 | ILE | A | 232 | 17.234 | 31.796 | 9.809 | 1.00 | 32.87 | C |
| ATOM | 1572 | CD1 | ILE | A | 232 | 17.895 | 30.699 | 8.996 | 1.00 | 33.81 | C |
| ATOM | 1573 | CG2 | ILE | A | 232 | 18.494 | 33.869 | 9.078 | 1.00 | 32.45 | C |
| ATOM | 1574 | N | LEU | A | 233 | 14.179 | 32.745 | 10.653 | 1.00 | 31.10 | N |
| ATOM | 1575 | CA | LEU | A | 233 | 12.895 | 32.045 | 10.697 | 1.00 | 30.98 | C |
| ATOM | 1576 | C | LEU | A | 233 | 11.705 | 33.011 | 10.636 | 1.00 | 31.26 | C |
| ATOM | 1577 | O | LEU | A | 233 | 10.732 | 32.762 | 9.920 | 1.00 | 30.66 | O |
| ATOM | 1578 | CB | LEU | A | 233 | 12.806 | 31.130 | 11.926 | 1.00 | 30.75 | C |
| ATOM | 1579 | CG | LEU | A | 233 | 13.704 | 29.883 | 11.901 | 1.00 | 30.29 | C |
| ATOM | 1580 | CD1 | LEU | A | 233 | 13.834 | 29.273 | 13.289 | 1.00 | 29.86 | C |
| ATOM | 1581 | CD2 | LEU | A | 233 | 13.189 | 28.862 | 10.899 | 1.00 | 29.92 | C |
| ATOM | 1582 | N | GLU | A | 234 | 11.803 | 34.111 | 11.381 | 1.00 | 31.82 | N |
| ATOM | 1583 | CA | GLU | A | 234 | 10.809 | 35.187 | 11.338 | 1.00 | 32.74 | C |
| ATOM | 1584 | C | GLU | A | 234 | 10.742 | 35.851 | 9.954 | 1.00 | 32.56 | C |
| ATOM | 1585 | O | GLU | A | 234 | 9.675 | 36.292 | 9.525 | 1.00 | 32.91 | O |
| ATOM | 1586 | CB | GLU | A | 234 | 11.073 | 36.223 | 12.441 | 1.00 | 32.88 | C |
| ATOM | 1587 | CG | GLU | A | 234 | 10.691 | 35.744 | 13.834 | 1.00 | 34.72 | C |
| ATOM | 1588 | CD | GLU | A | 234 | 11.373 | 36.523 | 14.953 | 1.00 | 38.13 | C |
| ATOM | 1589 | OE1 | GLU | A | 234 | 12.628 | 36.605 | 14.970 | 1.00 | 38.06 | O |
| ATOM | 1590 | OE2 | GLU | A | 234 | 10.647 | 37.048 | 15.836 | 1.00 | 38.86 | O |
| ATOM | 1591 | N | LYS | A | 235 | 11.875 | 35.890 | 9.255 | 1.00 | 32.60 | N |
| ATOM | 1592 | CA | LYS | A | 235 | 11.921 | 36.369 | 7.870 | 1.00 | 32.94 | C |
| ATOM | 1593 | C | LYS | A | 235 | 11.333 | 35.363 | 6.871 | 1.00 | 32.49 | C |
| ATOM | 1594 | O | LYS | A | 235 | 11.252 | 35.650 | 5.677 | 1.00 | 32.95 | O |
| ATOM | 1595 | CB | LYS | A | 235 | 13.361 | 36.698 | 7.460 | 1.00 | 33.46 | C |
| ATOM | 1596 | CG | LYS | A | 235 | 13.792 | 38.128 | 7.731 | 1.00 | 34.18 | C |
| ATOM | 1597 | CD | LYS | A | 235 | 15.036 | 38.161 | 8.614 | 1.00 | 35.32 | C |
| ATOM | 1598 | CE | LYS | A | 235 | 16.255 | 38.639 | 7.853 | 1.00 | 35.91 | C |
| ATOM | 1599 | NZ | LYS | A | 235 | 17.515 | 38.319 | 8.588 | 1.00 | 36.74 | N |
| ATOM | 1600 | N | GLY | A | 236 | 10.953 | 34.182 | 7.352 | 1.00 | 31.86 | N |
| ATOM | 1601 | CA | GLY | A | 236 | 10.312 | 33.174 | 6.521 | 1.00 | 30.53 | C |
| ATOM | 1602 | C | GLY | A | 236 | 11.255 | 32.178 | 5.862 | 1.00 | 29.96 | C |
| ATOM | 1603 | O | GLY | A | 236 | 10.830 | 31.393 | 5.007 | 1.00 | 30.10 | O |
| ATOM | 1604 | N | GLU | A | 237 | 12.528 | 32.206 | 6.249 | 1.00 | 28.50 | N |
| ATOM | 1605 | CA | GLU | A | 237 | 13.507 | 31.259 | 5.727 | 1.00 | 27.83 | C |
| ATOM | 1606 | C | GLU | A | 237 | 13.347 | 29.887 | 6.375 | 1.00 | 26.58 | C |
| ATOM | 1607 | O | GLU | A | 237 | 13.135 | 29.776 | 7.590 | 1.00 | 26.31 | O |
| ATOM | 1608 | CB | GLU | A | 237 | 14.933 | 31.750 | 5.966 | 1.00 | 28.59 | C |
| ATOM | 1609 | CG | GLU | A | 237 | 15.260 | 33.126 | 5.406 | 1.00 | 30.58 | C |
| ATOM | 1610 | CD | GLU | A | 237 | 16.732 | 33.256 | 5.089 | 1.00 | 32.61 | C |
| ATOM | 1611 | OE1 | GLU | A | 237 | 17.209 | 32.465 | 4.243 | 1.00 | 34.70 | O |
| ATOM | 1612 | OE2 | GLU | A | 237 | 17.414 | 34.118 | 5.690 | 1.00 | 32.10 | O |
| ATOM | 1613 | N | ARG | A | 238 | 13.460 | 28.850 | 5.555 | 1.00 | 24.84 | N |
| ATOM | 1614 | CA | ARG | A | 238 | 13.410 | 27.476 | 6.034 | 1.00 | 23.97 | C |

FIG. 5AA

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1615 | C | ARG | A | 238 | 14.554 | 26.674 | 5.420 | 1.00 | 23.40 | C |
| ATOM | 1616 | O | ARG | A | 238 | 15.214 | 27.139 | 4.500 | 1.00 | 23.59 | O |
| ATOM | 1617 | CB | ARG | A | 238 | 12.057 | 26.829 | 5.697 | 1.00 | 23.36 | C |
| ATOM | 1618 | CG | ARG | A | 238 | 10.844 | 27.460 | 6.369 | 1.00 | 22.61 | C |
| ATOM | 1619 | CD | ARG | A | 238 | 10.880 | 27.434 | 7.889 | 1.00 | 22.28 | C |
| ATOM | 1620 | NE | ARG | A | 238 | 9.650 | 27.959 | 8.479 | 1.00 | 21.42 | N |
| ATOM | 1621 | CZ | ARG | A | 238 | 9.473 | 29.212 | 8.887 | 1.00 | 21.46 | C |
| ATOM | 1622 | NH1 | ARG | A | 238 | 10.452 | 30.115 | 8.775 | 1.00 | 19.78 | N |
| ATOM | 1623 | NH2 | ARG | A | 238 | 8.307 | 29.561 | 9.422 | 1.00 | 20.88 | N |
| ATOM | 1624 | N | LEU | A | 239 | 14.788 | 25.477 | 5.951 | 1.00 | 23.06 | N |
| ATOM | 1625 | CA | LEU | A | 239 | 15.751 | 24.538 | 5.388 | 1.00 | 22.31 | C |
| ATOM | 1626 | C | LEU | A | 239 | 15.342 | 24.162 | 3.963 | 1.00 | 22.27 | C |
| ATOM | 1627 | O | LEU | A | 239 | 14.165 | 23.902 | 3.711 | 1.00 | 22.74 | O |
| ATOM | 1628 | CB | LEU | A | 239 | 15.829 | 23.278 | 6.264 | 1.00 | 21.98 | C |
| ATOM | 1629 | CG | LEU | A | 239 | 16.383 | 23.461 | 7.679 | 1.00 | 20.93 | C |
| ATOM | 1630 | CD1 | LEU | A | 239 | 15.787 | 22.448 | 8.656 | 1.00 | 17.59 | C |
| ATOM | 1631 | CD2 | LEU | A | 239 | 17.905 | 23.381 | 7.661 | 1.00 | 20.45 | C |
| ATOM | 1632 | N | PRO | A | 240 | 16.300 | 24.144 | 3.036 | 1.00 | 22.36 | N |
| ATOM | 1633 | CA | PRO | A | 240 | 16.015 | 23.875 | 1.614 | 1.00 | 22.32 | C |
| ATOM | 1634 | C | PRO | A | 240 | 15.571 | 22.436 | 1.315 | 1.00 | 22.70 | C |
| ATOM | 1635 | O | PRO | A | 240 | 15.832 | 21.539 | 2.113 | 1.00 | 23.10 | O |
| ATOM | 1636 | CB | PRO | A | 240 | 17.360 | 24.140 | 0.939 | 1.00 | 21.99 | C |
| ATOM | 1637 | CG | PRO | A | 240 | 18.369 | 23.919 | 2.015 | 1.00 | 22.25 | C |
| ATOM | 1638 | CD | PRO | A | 240 | 17.734 | 24.394 | 3.278 | 1.00 | 22.24 | C |
| ATOM | 1639 | N | GLN | A | 241 | 14.935 | 22.229 | 0.164 | 1.00 | 22.58 | N |
| ATOM | 1640 | CA | GLN | A | 241 | 14.434 | 20.919 | -0.221 | 1.00 | 23.36 | C |
| ATOM | 1641 | C | GLN | A | 241 | 15.578 | 19.939 | -0.504 | 1.00 | 23.53 | C |
| ATOM | 1642 | O | GLN | A | 241 | 16.468 | 20.228 | -1.300 | 1.00 | 23.49 | O |
| ATOM | 1643 | CB | GLN | A | 241 | 13.514 | 21.027 | -1.439 | 1.00 | 23.35 | C |
| ATOM | 1644 | CG | GLN | A | 241 | 12.769 | 19.740 | -1.769 | 1.00 | 25.02 | C |
| ATOM | 1645 | CD | GLN | A | 241 | 11.791 | 19.886 | -2.924 | 1.00 | 26.48 | C |
| ATOM | 1646 | OE1 | GLN | A | 241 | 11.402 | 20.996 | -3.278 | 1.00 | 27.61 | O |
| ATOM | 1647 | NE2 | GLN | A | 241 | 11.388 | 18.762 | -3.508 | 1.00 | 27.11 | N |
| ATOM | 1648 | N | PRO | A | 242 | 15.567 | 18.794 | 0.169 | 1.00 | 23.73 | N |
| ATOM | 1649 | CA | PRO | A | 242 | 16.552 | 17.747 | -0.104 | 1.00 | 23.94 | C |
| ATOM | 1650 | C | PRO | A | 242 | 16.316 | 17.155 | -1.494 | 1.00 | 23.79 | C |
| ATOM | 1651 | O | PRO | A | 242 | 15.167 | 16.913 | -1.859 | 1.00 | 23.48 | O |
| ATOM | 1652 | CB | PRO | A | 242 | 16.282 | 16.718 | 0.997 | 1.00 | 23.82 | C |
| ATOM | 1653 | CG | PRO | A | 242 | 15.553 | 17.498 | 2.038 | 1.00 | 24.29 | C |
| ATOM | 1654 | CD | PRO | A | 242 | 14.648 | 18.411 | 1.257 | 1.00 | 23.74 | C |
| ATOM | 1655 | N | PRO | A | 243 | 17.393 | 16.974 | -2.256 | 1.00 | 23.85 | N |
| ATOM | 1656 | CA | PRO | A | 243 | 17.339 | 16.405 | -3.615 | 1.00 | 24.02 | C |
| ATOM | 1657 | C | PRO | A | 243 | 16.460 | 15.166 | -3.792 | 1.00 | 23.91 | C |
| ATOM | 1658 | O | PRO | A | 243 | 15.828 | 15.050 | -4.833 | 1.00 | 24.44 | O |
| ATOM | 1659 | CB | PRO | A | 243 | 18.808 | 16.063 | -3.903 | 1.00 | 23.96 | C |
| ATOM | 1660 | CG | PRO | A | 243 | 19.573 | 17.090 | -3.133 | 1.00 | 23.87 | C |
| ATOM | 1661 | CD | PRO | A | 243 | 18.766 | 17.361 | -1.876 | 1.00 | 23.68 | C |
| ATOM | 1662 | N | ILE | A | 244 | 16.412 | 14.265 | -2.817 | 1.00 | 24.05 | N |
| ATOM | 1663 | CA | ILE | A | 244 | 15.612 | 13.038 | -2.956 | 1.00 | 24.12 | C |
| ATOM | 1664 | C | ILE | A | 244 | 14.105 | 13.238 | -2.743 | 1.00 | 24.71 | C |
| ATOM | 1665 | O | ILE | A | 244 | 13.318 | 12.339 | -3.043 | 1.00 | 24.49 | O |
| ATOM | 1666 | CB | ILE | A | 244 | 16.141 | 11.891 | -2.029 | 1.00 | 23.86 | C |
| ATOM | 1667 | CG1 | ILE | A | 244 | 16.078 | 12.297 | -0.554 | 1.00 | 23.91 | C |
| ATOM | 1668 | CD1 | ILE | A | 244 | 15.788 | 11.139 | 0.386 | 1.00 | 25.03 | C |
| ATOM | 1669 | CG2 | ILE | A | 244 | 17.561 | 11.446 | -2.445 | 1.00 | 22.93 | C |
| ATOM | 1670 | N | CYS | A | 245 | 13.710 | 14.407 | -2.231 | 1.00 | 25.35 | N |
| ATOM | 1671 | CA | CYS | A | 245 | 12.336 | 14.634 | -1.768 | 1.00 | 26.36 | C |
| ATOM | 1672 | C | CYS | A | 245 | 11.408 | 15.120 | -2.867 | 1.00 | 26.04 | C |
| ATOM | 1673 | O | CYS | A | 245 | 11.696 | 16.123 | -3.512 | 1.00 | 26.37 | O |
| ATOM | 1674 | CB | CYS | A | 245 | 12.316 | 15.675 | -0.643 | 1.00 | 26.68 | C |

FIG. 5BB

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1675 | SG | CYS | A | 245 | 12.891 | 15.079 | 0.956 | 1.00 | 29.71 | S |
| ATOM | 1676 | N | THR | A | 246 | 10.286 | 14.430 | -3.065 | 1.00 | 25.97 | N |
| ATOM | 1677 | CA | THR | A | 246 | 9.234 | 14.961 | -3.930 | 1.00 | 26.41 | C |
| ATOM | 1678 | C | THR | A | 246 | 8.598 | 16.163 | -3.259 | 1.00 | 26.53 | C |
| ATOM | 1679 | O | THR | A | 246 | 8.764 | 16.379 | -2.049 | 1.00 | 26.34 | O |
| ATOM | 1680 | CB | THR | A | 246 | 8.146 | 13.917 | -4.252 | 1.00 | 26.72 | C |
| ATOM | 1681 | OG1 | THR | A | 246 | 7.689 | 13.291 | -3.043 | 1.00 | 27.60 | O |
| ATOM | 1682 | CG2 | THR | A | 246 | 8.716 | 12.776 | -5.097 | 1.00 | 26.65 | C |
| ATOM | 1683 | N | ILE | A | 247 | 7.867 | 16.948 | -4.047 | 1.00 | 26.79 | N |
| ATOM | 1684 | CA | ILE | A | 247 | 7.208 | 18.146 | -3.539 | 1.00 | 26.43 | C |
| ATOM | 1685 | C | ILE | A | 247 | 6.324 | 17.803 | -2.339 | 1.00 | 26.30 | C |
| ATOM | 1686 | O | ILE | A | 247 | 6.293 | 18.547 | -1.366 | 1.00 | 26.86 | O |
| ATOM | 1687 | CB | ILE | A | 247 | 6.419 | 18.864 | -4.668 | 1.00 | 26.87 | C |
| ATOM | 1688 | CG1 | ILE | A | 247 | 6.049 | 20.293 | -4.248 | 1.00 | 26.78 | C |
| ATOM | 1689 | CG2 | ILE | A | 247 | 5.185 | 18.056 | -5.098 | 1.00 | 26.73 | C |
| ATOM | 1690 | N | ASP | A | 248 | 5.652 | 16.653 | -2.403 | 1.00 | 25.73 | N |
| ATOM | 1691 | CA | ASP | A | 248 | 4.764 | 16.192 | -1.344 | 1.00 | 25.42 | C |
| ATOM | 1692 | C | ASP | A | 248 | 5.463 | 16.044 | 0.012 | 1.00 | 25.11 | C |
| ATOM | 1693 | O | ASP | A | 248 | 4.939 | 16.510 | 1.034 | 1.00 | 25.20 | O |
| ATOM | 1694 | CB | ASP | A | 248 | 4.107 | 14.873 | -1.743 | 1.00 | 26.14 | C |
| ATOM | 1695 | CG | ASP | A | 248 | 3.328 | 14.978 | -3.053 | 1.00 | 27.68 | C |
| ATOM | 1696 | OD1 | ASP | A | 248 | 3.959 | 14.972 | -4.136 | 1.00 | 28.63 | O |
| ATOM | 1697 | OD2 | ASP | A | 248 | 2.085 | 15.070 | -3.095 | 1.00 | 27.81 | O |
| ATOM | 1698 | N | VAL | A | 249 | 6.634 | 15.402 | 0.013 | 1.00 | 23.56 | N |
| ATOM | 1699 | CA | VAL | A | 249 | 7.411 | 15.176 | 1.241 | 1.00 | 22.27 | C |
| ATOM | 1700 | C | VAL | A | 249 | 7.865 | 16.503 | 1.852 | 1.00 | 21.34 | C |
| ATOM | 1701 | O | VAL | A | 249 | 7.631 | 16.755 | 3.033 | 1.00 | 20.14 | O |
| ATOM | 1702 | CB | VAL | A | 249 | 8.615 | 14.206 | 1.002 | 1.00 | 22.04 | C |
| ATOM | 1703 | CG1 | VAL | A | 249 | 9.521 | 14.159 | 2.203 | 1.00 | 21.97 | C |
| ATOM | 1704 | CG2 | VAL | A | 249 | 8.111 | 12.801 | 0.705 | 1.00 | 21.72 | C |
| ATOM | 1705 | N | TYR | A | 250 | 8.472 | 17.359 | 1.029 | 1.00 | 21.08 | N |
| ATOM | 1706 | CA | TYR | A | 250 | 8.893 | 18.688 | 1.466 | 1.00 | 21.47 | C |
| ATOM | 1707 | C | TYR | A | 250 | 7.743 | 19.557 | 2.004 | 1.00 | 21.79 | C |
| ATOM | 1708 | O | TYR | A | 250 | 7.948 | 20.326 | 2.948 | 1.00 | 21.21 | O |
| ATOM | 1709 | CB | TYR | A | 250 | 9.648 | 19.431 | 0.352 | 1.00 | 21.05 | C |
| ATOM | 1710 | CG | TYR | A | 250 | 10.332 | 20.706 | 0.821 | 1.00 | 20.50 | C |
| ATOM | 1711 | CD1 | TYR | A | 250 | 10.005 | 21.949 | 0.257 | 1.00 | 20.75 | C |
| ATOM | 1712 | CE1 | TYR | A | 250 | 10.624 | 23.123 | 0.679 | 1.00 | 19.33 | C |
| ATOM | 1713 | CZ | TYR | A | 250 | 11.577 | 23.061 | 1.677 | 1.00 | 20.22 | C |
| ATOM | 1714 | OH | TYR | A | 250 | 12.188 | 24.212 | 2.103 | 1.00 | 20.81 | O |
| ATOM | 1715 | CE2 | TYR | A | 250 | 11.922 | 21.840 | 2.257 | 1.00 | 20.09 | C |
| ATOM | 1716 | CD2 | TYR | A | 250 | 11.294 | 20.676 | 1.830 | 1.00 | 19.31 | C |
| ATOM | 1717 | N | MET | A | 251 | 6.550 | 19.434 | 1.409 | 1.00 | 22.18 | N |
| ATOM | 1718 | CA | MET | A | 251 | 5.381 | 20.195 | 1.866 | 1.00 | 23.03 | C |
| ATOM | 1719 | C | MET | A | 251 | 5.039 | 19.834 | 3.308 | 1.00 | 22.94 | C |
| ATOM | 1720 | O | MET | A | 251 | 4.781 | 20.721 | 4.123 | 1.00 | 22.97 | O |
| ATOM | 1721 | CB | MET | A | 251 | 4.162 | 20.010 | 0.946 | 1.00 | 23.69 | C |
| ATOM | 1722 | CG | MET | A | 251 | 4.350 | 20.535 | -0.480 | 1.00 | 26.38 | C |
| ATOM | 1723 | SD | MET | A | 251 | 3.173 | 21.801 | -1.043 | 1.00 | 31.94 | S |
| ATOM | 1724 | CE | MET | A | 251 | 4.311 | 23.007 | -1.795 | 1.00 | 29.59 | C |
| ATOM | 1725 | N | ILE | A | 252 | 5.075 | 18.538 | 3.625 | 1.00 | 22.98 | N |
| ATOM | 1726 | CA | ILE | A | 252 | 4.890 | 18.075 | 5.004 | 1.00 | 23.33 | C |
| ATOM | 1727 | C | ILE | A | 252 | 5.924 | 18.672 | 5.960 | 1.00 | 22.47 | C |
| ATOM | 1728 | O | ILE | A | 252 | 5.572 | 19.117 | 7.047 | 1.00 | 22.57 | O |
| ATOM | 1729 | CB | ILE | A | 252 | 4.890 | 16.525 | 5.083 | 1.00 | 23.89 | C |
| ATOM | 1730 | CG1 | ILE | A | 252 | 3.682 | 15.957 | 4.333 | 1.00 | 24.47 | C |
| ATOM | 1731 | CD1 | ILE | A | 252 | 3.784 | 14.480 | 4.037 | 1.00 | 26.22 | C |
| ATOM | 1732 | CG2 | ILE | A | 252 | 4.868 | 16.065 | 6.534 | 1.00 | 24.02 | C |
| ATOM | 1733 | N | MET | A | 253 | 7.188 | 18.693 | 5.545 | 1.00 | 22.24 | N |
| ATOM | 1734 | CA | MET | A | 253 | 8.258 | 19.315 | 6.340 | 1.00 | 22.01 | C |

FIG. 5CC

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1735 | C | MET | A | 253 | 8.011 | 20.803 | 6.558 | 1.00 | 20.97 | C |
| ATOM | 1736 | O | MET | A | 253 | 8.200 | 21.312 | 7.654 | 1.00 | 20.96 | O |
| ATOM | 1737 | CB | MET | A | 253 | 9.619 | 19.148 | 5.665 | 1.00 | 22.41 | C |
| ATOM | 1738 | CG | MET | A | 253 | 10.166 | 17.732 | 5.624 | 1.00 | 23.98 | C |
| ATOM | 1739 | SD | MET | A | 253 | 11.819 | 17.718 | 4.863 | 1.00 | 25.73 | S |
| ATOM | 1740 | CE | MET | A | 253 | 11.523 | 16.543 | 3.614 | 1.00 | 24.41 | C |
| ATOM | 1741 | N | VAL | A | 254 | 7.613 | 21.499 | 5.498 | 1.00 | 20.48 | N |
| ATOM | 1742 | CA | VAL | A | 254 | 7.333 | 22.938 | 5.576 | 1.00 | 19.92 | C |
| ATOM | 1743 | C | VAL | A | 254 | 6.183 | 23.200 | 6.554 | 1.00 | 19.02 | C |
| ATOM | 1744 | O | VAL | A | 254 | 6.271 | 24.094 | 7.396 | 1.00 | 17.82 | O |
| ATOM | 1745 | CB | VAL | A | 254 | 7.070 | 23.554 | 4.163 | 1.00 | 19.97 | C |
| ATOM | 1746 | CG1 | VAL | A | 254 | 6.283 | 24.861 | 4.246 | 1.00 | 20.08 | C |
| ATOM | 1747 | CG2 | VAL | A | 254 | 8.384 | 23.795 | 3.455 | 1.00 | 20.32 | C |
| ATOM | 1748 | N | LYS | A | 255 | 5.130 | 22.389 | 6.451 | 1.00 | 18.68 | N |
| ATOM | 1749 | CA | LYS | A | 255 | 4.010 | 22.435 | 7.393 | 1.00 | 18.62 | C |
| ATOM | 1750 | C | LYS | A | 255 | 4.456 | 22.338 | 8.862 | 1.00 | 18.01 | C |
| ATOM | 1751 | O | LYS | A | 255 | 3.885 | 22.995 | 9.717 | 1.00 | 16.95 | O |
| ATOM | 1752 | CB | LYS | A | 255 | 2.987 | 21.333 | 7.084 | 1.00 | 18.90 | C |
| ATOM | 1753 | CG | LYS | A | 255 | 2.148 | 21.558 | 5.825 | 1.00 | 20.18 | C |
| ATOM | 1754 | N | CYS | A | 256 | 5.470 | 21.519 | 9.144 | 1.00 | 17.79 | N |
| ATOM | 1755 | CA | CYS | A | 256 | 5.976 | 21.362 | 10.508 | 1.00 | 18.81 | C |
| ATOM | 1756 | C | CYS | A | 256 | 6.630 | 22.638 | 11.057 | 1.00 | 19.25 | C |
| ATOM | 1757 | O | CYS | A | 256 | 6.810 | 22.775 | 12.270 | 1.00 | 19.01 | O |
| ATOM | 1758 | CB | CYS | A | 256 | 6.969 | 20.195 | 10.598 | 1.00 | 18.67 | C |
| ATOM | 1759 | SG | CYS | A | 256 | 6.260 | 18.549 | 10.306 | 1.00 | 19.41 | S |
| ATOM | 1760 | N | TRP | A | 257 | 6.981 | 23.559 | 10.159 | 1.00 | 19.82 | N |
| ATOM | 1761 | CA | TRP | A | 257 | 7.705 | 24.779 | 10.516 | 1.00 | 20.64 | C |
| ATOM | 1762 | C | TRP | A | 257 | 6.875 | 26.066 | 10.373 | 1.00 | 21.80 | C |
| ATOM | 1763 | O | TRP | A | 257 | 7.437 | 27.155 | 10.237 | 1.00 | 22.16 | O |
| ATOM | 1764 | CB | TRP | A | 257 | 8.997 | 24.909 | 9.696 | 1.00 | 19.37 | C |
| ATOM | 1765 | CG | TRP | A | 257 | 9.918 | 23.732 | 9.765 | 1.00 | 18.88 | C |
| ATOM | 1766 | CD1 | TRP | A | 257 | 10.209 | 22.974 | 10.866 | 1.00 | 18.24 | C |
| ATOM | 1767 | NE1 | TRP | A | 257 | 11.100 | 21.983 | 10.536 | 1.00 | 18.05 | N |
| ATOM | 1768 | CE2 | TRP | A | 257 | 11.399 | 22.077 | 9.202 | 1.00 | 18.42 | C |
| ATOM | 1769 | CD2 | TRP | A | 257 | 10.678 | 23.174 | 8.685 | 1.00 | 18.49 | C |
| ATOM | 1770 | CE3 | TRP | A | 257 | 10.815 | 23.482 | 7.323 | 1.00 | 18.38 | C |
| ATOM | 1771 | CZ3 | TRP | A | 257 | 11.661 | 22.703 | 6.537 | 1.00 | 18.42 | C |
| ATOM | 1772 | CH2 | TRP | A | 257 | 12.370 | 21.623 | 7.087 | 1.00 | 18.16 | C |
| ATOM | 1773 | CZ2 | TRP | A | 257 | 12.251 | 21.295 | 8.412 | 1.00 | 18.72 | C |
| ATOM | 1774 | N | MET | A | 258 | 5.551 | 25.944 | 10.391 | 1.00 | 23.26 | N |
| ATOM | 1775 | CA | MET | A | 258 | 4.673 | 27.118 | 10.460 | 1.00 | 24.83 | C |
| ATOM | 1776 | C | MET | A | 258 | 4.920 | 27.857 | 11.768 | 1.00 | 25.27 | C |
| ATOM | 1777 | O | MET | A | 258 | 5.149 | 27.225 | 12.815 | 1.00 | 25.71 | O |
| ATOM | 1778 | CB | MET | A | 258 | 3.200 | 26.719 | 10.411 | 1.00 | 25.26 | C |
| ATOM | 1779 | CG | MET | A | 258 | 2.860 | 25.612 | 9.441 | 1.00 | 27.53 | C |
| ATOM | 1780 | SD | MET | A | 258 | 2.500 | 26.199 | 7.794 | 1.00 | 31.59 | S |
| ATOM | 1781 | CE | MET | A | 258 | 0.844 | 26.895 | 8.011 | 1.00 | 30.46 | C |
| ATOM | 1782 | N | ILE | A | 259 | 4.880 | 29.187 | 11.708 | 1.00 | 25.59 | N |
| ATOM | 1783 | CA | ILE | A | 259 | 4.985 | 30.022 | 12.906 | 1.00 | 25.77 | C |
| ATOM | 1784 | C | ILE | A | 259 | 3.831 | 29.718 | 13.858 | 1.00 | 25.67 | C |
| ATOM | 1785 | O | ILE | A | 259 | 4.033 | 29.623 | 15.060 | 1.00 | 26.34 | O |
| ATOM | 1786 | CB | ILE | A | 259 | 4.979 | 31.533 | 12.545 | 1.00 | 26.09 | C |
| ATOM | 1787 | CG1 | ILE | A | 259 | 5.994 | 31.854 | 11.439 | 1.00 | 26.19 | C |
| ATOM | 1788 | CD1 | ILE | A | 259 | 7.412 | 32.100 | 11.901 | 1.00 | 27.92 | C |
| ATOM | 1789 | CG2 | ILE | A | 259 | 5.183 | 32.391 | 13.798 | 1.00 | 26.48 | C |
| ATOM | 1790 | N | ASP | A | 260 | 2.625 | 29.581 | 13.310 | 1.00 | 25.91 | N |
| ATOM | 1791 | CA | ASP | A | 260 | 1.438 | 29.220 | 14.085 | 1.00 | 26.00 | C |
| ATOM | 1792 | C | ASP | A | 260 | 1.470 | 27.726 | 14.433 | 1.00 | 25.77 | C |
| ATOM | 1793 | O | ASP | A | 260 | 1.267 | 26.868 | 13.567 | 1.00 | 25.19 | O |
| ATOM | 1794 | CB | ASP | A | 260 | 0.176 | 29.570 | 13.288 | 1.00 | 26.40 | C |

FIG. SDD

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1795 | CG | ASP | A | 260 | -1.109 | 29.266 | 14.041 | 1.00 | 27.75 | C |
| ATOM | 1796 | OD1 | ASP | A | 260 | -1.144 | 29.388 | 15.282 | 1.00 | 30.06 | O |
| ATOM | 1797 | OD2 | ASP | A | 260 | -2.154 | 28.909 | 13.464 | 1.00 | 29.15 | O |
| ATOM | 1798 | N | ALA | A | 261 | 1.734 | 27.431 | 15.704 | 1.00 | 25.81 | N |
| ATOM | 1799 | CA | ALA | A | 261 | 1.924 | 26.058 | 16.187 | 1.00 | 25.67 | C |
| ATOM | 1800 | C | ALA | A | 261 | 0.717 | 25.161 | 15.937 | 1.00 | 26.09 | C |
| ATOM | 1801 | O | ALA | A | 261 | 0.865 | 23.971 | 15.666 | 1.00 | 26.38 | O |
| ATOM | 1802 | CB | ALA | A | 261 | 2.286 | 26.066 | 17.665 | 1.00 | 25.12 | C |
| ATOM | 1803 | N | ASP | A | 262 | -0.474 | 25.746 | 16.019 | 1.00 | 26.76 | N |
| ATOM | 1804 | CA | ASP | A | 262 | -1.721 | 25.028 | 15.794 | 1.00 | 27.09 | C |
| ATOM | 1805 | C | ASP | A | 262 | -1.980 | 24.677 | 14.334 | 1.00 | 26.53 | C |
| ATOM | 1806 | O | ASP | A | 262 | -2.850 | 23.854 | 14.040 | 1.00 | 25.86 | O |
| ATOM | 1807 | CB | ASP | A | 262 | -2.903 | 25.837 | 16.341 | 1.00 | 28.40 | C |
| ATOM | 1808 | CG | ASP | A | 262 | -3.212 | 25.496 | 17.780 | 1.00 | 29.96 | C |
| ATOM | 1809 | OD1 | ASP | A | 262 | -3.772 | 24.403 | 18.031 | 1.00 | 31.76 | O |
| ATOM | 1810 | OD2 | ASP | A | 262 | -2.916 | 26.251 | 18.724 | 1.00 | 31.29 | O |
| ATOM | 1811 | N | SER | A | 263 | -1.247 | 25.304 | 13.417 | 1.00 | 25.76 | N |
| ATOM | 1812 | CA | SER | A | 263 | -1.411 | 24.967 | 12.006 | 1.00 | 25.84 | C |
| ATOM | 1813 | C | SER | A | 263 | -0.391 | 23.924 | 11.519 | 1.00 | 24.48 | C |
| ATOM | 1814 | O | SER | A | 263 | -0.395 | 23.545 | 10.353 | 1.00 | 24.57 | O |
| ATOM | 1815 | CB | SER | A | 263 | -1.425 | 26.221 | 11.122 | 1.00 | 25.90 | C |
| ATOM | 1816 | OG | SER | A | 263 | -0.113 | 26.698 | 10.925 | 1.00 | 29.08 | O |
| ATOM | 1817 | N | ARG | A | 264 | 0.472 | 23.468 | 12.424 | 1.00 | 23.19 | N |
| ATOM | 1818 | CA | ARG | A | 264 | 1.396 | 22.378 | 12.136 | 1.00 | 21.98 | C |
| ATOM | 1819 | C | ARG | A | 264 | 0.633 | 21.051 | 12.218 | 1.00 | 21.72 | C |
| ATOM | 1820 | O | ARG | A | 264 | -0.353 | 20.943 | 12.961 | 1.00 | 21.71 | O |
| ATOM | 1821 | CB | ARG | A | 264 | 2.543 | 22.369 | 13.147 | 1.00 | 21.66 | C |
| ATOM | 1822 | CG | ARG | A | 264 | 3.498 | 23.553 | 13.058 | 1.00 | 20.71 | C |
| ATOM | 1823 | CD | ARG | A | 264 | 4.437 | 23.688 | 14.270 | 1.00 | 19.74 | C |
| ATOM | 1824 | NE | ARG | A | 264 | 4.875 | 25.072 | 14.446 | 1.00 | 19.73 | N |
| ATOM | 1825 | CZ | ARG | A | 264 | 5.352 | 25.592 | 15.574 | 1.00 | 19.18 | C |
| ATOM | 1826 | NH1 | ARG | A | 264 | 5.699 | 26.871 | 15.596 | 1.00 | 17.68 | N |
| ATOM | 1827 | NH2 | ARG | A | 264 | 5.488 | 24.850 | 16.674 | 1.00 | 16.00 | N |
| ATOM | 1828 | N | PRO | A | 265 | 1.072 | 20.042 | 11.468 | 1.00 | 21.06 | N |
| ATOM | 1829 | CA | PRO | A | 265 | 0.467 | 18.705 | 11.556 | 1.00 | 20.80 | C |
| ATOM | 1830 | C | PRO | A | 265 | 0.490 | 18.155 | 12.974 | 1.00 | 20.48 | C |
| ATOM | 1831 | O | PRO | A | 265 | 1.320 | 18.563 | 13.778 | 1.00 | 21.30 | O |
| ATOM | 1832 | CB | PRO | A | 265 | 1.379 | 17.847 | 10.680 | 1.00 | 20.71 | C |
| ATOM | 1833 | CG | PRO | A | 265 | 2.031 | 18.810 | 9.737 | 1.00 | 21.16 | C |
| ATOM | 1834 | CD | PRO | A | 265 | 2.173 | 20.093 | 10.487 | 1.00 | 21.05 | C |
| ATOM | 1835 | N | LYS | A | 266 | -0.424 | 17.245 | 13.275 | 1.00 | 20.19 | N |
| ATOM | 1836 | CA | LYS | A | 266 | -0.376 | 16.493 | 14.512 | 1.00 | 20.12 | C |
| ATOM | 1837 | C | LYS | A | 266 | 0.402 | 15.225 | 14.248 | 1.00 | 19.65 | C |
| ATOM | 1838 | O | LYS | A | 266 | 0.420 | 14.734 | 13.108 | 1.00 | 20.28 | O |
| ATOM | 1839 | CB | LYS | A | 266 | -1.788 | 16.142 | 14.987 | 1.00 | 20.90 | C |
| ATOM | 1840 | CG | LYS | A | 266 | -2.651 | 17.353 | 15.392 | 1.00 | 22.35 | C |
| ATOM | 1841 | CD | LYS | A | 266 | -2.036 | 18.159 | 16.531 | 1.00 | 24.13 | C |
| ATOM | 1842 | CE | LYS | A | 266 | -2.159 | 17.420 | 17.871 | 1.00 | 25.87 | C |
| ATOM | 1843 | NZ | LYS | A | 266 | -1.152 | 17.916 | 18.880 | 1.00 | 27.42 | N |
| ATOM | 1844 | N | PHE | A | 267 | 1.042 | 14.688 | 15.283 | 1.00 | 18.25 | N |
| ATOM | 1845 | CA | PHE | A | 267 | 1.741 | 13.410 | 15.148 | 1.00 | 17.73 | C |
| ATOM | 1846 | C | PHE | A | 267 | 0.828 | 12.287 | 14.621 | 1.00 | 17.91 | C |
| ATOM | 1847 | O | PHE | A | 267 | 1.235 | 11.539 | 13.739 | 1.00 | 18.09 | O |
| ATOM | 1848 | CB | PHE | A | 267 | 2.474 | 13.018 | 16.448 | 1.00 | 16.62 | C |
| ATOM | 1849 | CG | PHE | A | 267 | 3.757 | 13.786 | 16.675 | 1.00 | 14.86 | C |
| ATOM | 1850 | CD1 | PHE | A | 267 | 4.807 | 13.717 | 15.754 | 1.00 | 14.57 | C |
| ATOM | 1851 | CE1 | PHE | A | 267 | 5.998 | 14.424 | 15.956 | 1.00 | 13.52 | C |
| ATOM | 1852 | CZ | PHE | A | 267 | 6.137 | 15.226 | 17.097 | 1.00 | 13.45 | C |
| ATOM | 1853 | CE2 | PHE | A | 267 | 5.092 | 15.295 | 18.021 | 1.00 | 13.45 | C |
| ATOM | 1854 | CD2 | PHE | A | 267 | 3.916 | 14.581 | 17.806 | 1.00 | 13.41 | C |

FIG. SEE

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1855 | N | ARG | A | 268 | -0.404 | 12.196 | 15.123 | 1.00 | 18.54 | N |
| ATOM | 1856 | CA | ARG | A | 268 | -1.369 | 11.209 | 14.618 | 1.00 | 19.41 | C |
| ATOM | 1857 | C | ARG | A | 268 | -1.572 | 11.333 | 13.107 | 1.00 | 20.26 | C |
| ATOM | 1858 | O | ARG | A | 268 | -1.692 | 10.321 | 12.411 | 1.00 | 20.90 | O |
| ATOM | 1859 | CB | ARG | A | 268 | -2.717 | 11.319 | 15.335 | 1.00 | 18.84 | C |
| ATOM | 1860 | N | GLU | A | 269 | -1.597 | 12.576 | 12.620 | 1.00 | 20.30 | N |
| ATOM | 1861 | CA | GLU | A | 269 | -1.732 | 12.878 | 11.199 | 1.00 | 20.68 | C |
| ATOM | 1862 | C | GLU | A | 269 | -0.485 | 12.454 | 10.423 | 1.00 | 20.10 | C |
| ATOM | 1863 | O | GLU | A | 269 | -0.593 | 11.797 | 9.390 | 1.00 | 20.32 | O |
| ATOM | 1864 | CB | GLU | A | 269 | -2.010 | 14.373 | 10.988 | 1.00 | 20.61 | C |
| ATOM | 1865 | CG | GLU | A | 269 | -3.489 | 14.737 | 10.996 | 1.00 | 23.22 | C |
| ATOM | 1866 | CD | GLU | A | 269 | -3.814 | 16.047 | 11.720 | 1.00 | 26.05 | C |
| ATOM | 1867 | OE1 | GLU | A | 269 | -3.074 | 17.057 | 11.576 | 1.00 | 24.55 | O |
| ATOM | 1868 | OE2 | GLU | A | 269 | -4.852 | 16.072 | 12.430 | 1.00 | 27.97 | O |
| ATOM | 1869 | N | LEU | A | 270 | 0.691 | 12.825 | 10.936 | 1.00 | 19.58 | N |
| ATOM | 1870 | CA | LEU | A | 270 | 1.980 | 12.437 | 10.350 | 1.00 | 18.51 | C |
| ATOM | 1871 | C | LEU | A | 270 | 2.174 | 10.910 | 10.284 | 1.00 | 18.07 | C |
| ATOM | 1872 | O | LEU | A | 270 | 2.736 | 10.387 | 9.309 | 1.00 | 17.45 | O |
| ATOM | 1873 | CB | LEU | A | 270 | 3.143 | 13.090 | 11.107 | 1.00 | 18.03 | C |
| ATOM | 1874 | CG | LEU | A | 270 | 3.213 | 14.623 | 11.076 | 1.00 | 18.05 | C |
| ATOM | 1875 | CD1 | LEU | A | 270 | 4.173 | 15.150 | 12.143 | 1.00 | 17.10 | C |
| ATOM | 1876 | CD2 | LEU | A | 270 | 3.627 | 15.121 | 9.698 | 1.00 | 16.86 | C |
| ATOM | 1877 | N | ILE | A | 271 | 1.709 | 10.201 | 11.310 | 1.00 | 17.28 | N |
| ATOM | 1878 | CA | ILE | A | 271 | 1.689 | 8.741 | 11.247 | 1.00 | 17.15 | C |
| ATOM | 1879 | C | ILE | A | 271 | 0.950 | 8.304 | 9.981 | 1.00 | 17.61 | C |
| ATOM | 1880 | O | ILE | A | 271 | 1.530 | 7.618 | 9.146 | 1.00 | 18.33 | O |
| ATOM | 1881 | CB | ILE | A | 271 | 1.048 | 8.110 | 12.502 | 1.00 | 16.19 | C |
| ATOM | 1882 | CG1 | ILE | A | 271 | 1.932 | 8.323 | 13.735 | 1.00 | 15.11 | C |
| ATOM | 1883 | CD1 | ILE | A | 271 | 1.247 | 7.991 | 15.067 | 1.00 | 14.36 | C |
| ATOM | 1884 | CG2 | ILE | A | 271 | 0.805 | 6.627 | 12.279 | 1.00 | 15.98 | C |
| ATOM | 1885 | N | ILE | A | 272 | -0.303 | 8.738 | 9.830 | 1.00 | 17.87 | N |
| ATOM | 1886 | CA | ILE | A | 272 | -1.154 | 8.344 | 8.700 | 1.00 | 18.15 | C |
| ATOM | 1887 | C | ILE | A | 272 | -0.525 | 8.716 | 7.355 | 1.00 | 18.72 | C |
| ATOM | 1888 | O | ILE | A | 272 | -0.428 | 7.872 | 6.455 | 1.00 | 18.78 | O |
| ATOM | 1889 | CB | ILE | A | 272 | -2.581 | 8.980 | 8.837 | 1.00 | 18.38 | C |
| ATOM | 1890 | CG1 | ILE | A | 272 | -3.384 | 8.283 | 9.938 | 1.00 | 17.29 | C |
| ATOM | 1891 | CD1 | ILE | A | 272 | -4.382 | 9.213 | 10.642 | 1.00 | 17.41 | C |
| ATOM | 1892 | CG2 | ILE | A | 272 | -3.352 | 8.972 | 7.488 | 1.00 | 17.05 | C |
| ATOM | 1893 | N | GLU | A | 273 | -0.085 | 9.970 | 7.244 | 1.00 | 19.24 | N |
| ATOM | 1894 | CA | GLU | A | 273 | 0.481 | 10.511 | 6.007 | 1.00 | 19.84 | C |
| ATOM | 1895 | C | GLU | A | 273 | 1.727 | 9.768 | 5.547 | 1.00 | 20.65 | C |
| ATOM | 1896 | O | GLU | A | 273 | 1.804 | 9.342 | 4.395 | 1.00 | 21.30 | O |
| ATOM | 1897 | CB | GLU | A | 273 | 0.799 | 11.999 | 6.166 | 1.00 | 19.57 | C |
| ATOM | 1898 | N | PHE | A | 274 | 2.701 | 9.621 | 6.448 | 1.00 | 20.98 | N |
| ATOM | 1899 | CA | PHE | A | 274 | 3.950 | 8.946 | 6.125 | 1.00 | 21.08 | C |
| ATOM | 1900 | C | PHE | A | 274 | 3.741 | 7.445 | 5.886 | 1.00 | 21.17 | C |
| ATOM | 1901 | O | PHE | A | 274 | 4.391 | 6.854 | 5.023 | 1.00 | 20.52 | O |
| ATOM | 1902 | CB | PHE | A | 274 | 5.008 | 9.207 | 7.204 | 1.00 | 21.30 | C |
| ATOM | 1903 | CG | PHE | A | 274 | 5.849 | 10.425 | 6.941 | 1.00 | 21.25 | C |
| ATOM | 1904 | CD1 | PHE | A | 274 | 6.830 | 10.409 | 5.953 | 1.00 | 22.11 | C |
| ATOM | 1905 | CE1 | PHE | A | 274 | 7.614 | 11.549 | 5.702 | 1.00 | 22.74 | C |
| ATOM | 1906 | CZ | PHE | A | 274 | 7.414 | 12.713 | 6.455 | 1.00 | 21.83 | C |
| ATOM | 1907 | CE2 | PHE | A | 274 | 6.433 | 12.731 | 7.443 | 1.00 | 22.09 | C |
| ATOM | 1908 | CD2 | PHE | A | 274 | 5.660 | 11.591 | 7.680 | 1.00 | 21.68 | C |
| ATOM | 1909 | N | SER | A | 275 | 2.819 | 6.840 | 6.634 | 1.00 | 21.59 | N |
| ATOM | 1910 | CA | SER | A | 275 | 2.429 | 5.452 | 6.383 | 1.00 | 22.53 | C |
| ATOM | 1911 | C | SER | A | 275 | 1.900 | 5.240 | 4.960 | 1.00 | 23.05 | C |
| ATOM | 1912 | O | SER | A | 275 | 2.218 | 4.238 | 4.324 | 1.00 | 22.60 | O |
| ATOM | 1913 | CB | SER | A | 275 | 1.398 | 4.983 | 7.399 | 1.00 | 22.33 | C |
| ATOM | 1914 | OG | SER | A | 275 | 1.943 | 5.020 | 8.701 | 1.00 | 23.66 | O |

FIG. 5FF

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1915 | N | LYS | A | 276 | 1.107 | 6.188 | 4.462 | 1.00 | 24.02 | N |
| ATOM | 1916 | CA | LYS | A | 276 | 0.613 | 6.119 | 3.087 | 1.00 | 25.17 | C |
| ATOM | 1917 | C | LYS | A | 276 | 1.784 | 6.110 | 2.101 | 1.00 | 25.09 | C |
| ATOM | 1918 | O | LYS | A | 276 | 1.780 | 5.346 | 1.134 | 1.00 | 25.11 | O |
| ATOM | 1919 | CB | LYS | A | 276 | -0.336 | 7.284 | 2.792 | 1.00 | 25.75 | C |
| ATOM | 1920 | CG | LYS | A | 276 | -0.946 | 7.283 | 1.386 | 1.00 | 27.13 | C |
| ATOM | 1921 | CD | LYS | A | 276 | -0.582 | 8.558 | 0.621 | 1.00 | 29.40 | C |
| ATOM | 1922 | CE | LYS | A | 276 | -1.405 | 9.754 | 1.092 | 1.00 | 30.40 | C |
| ATOM | 1923 | NZ | LYS | A | 276 | -0.533 | 10.932 | 1.363 | 1.00 | 31.80 | N |
| ATOM | 1924 | N | MET | A | 277 | 2.781 | 6.951 | 2.373 | 1.00 | 25.24 | N |
| ATOM | 1925 | CA | MET | A | 277 | 3.975 | 7.070 | 1.534 | 1.00 | 25.11 | C |
| ATOM | 1926 | C | MET | A | 277 | 4.883 | 5.849 | 1.642 | 1.00 | 25.40 | C |
| ATOM | 1927 | O | MET | A | 277 | 5.548 | 5.474 | 0.667 | 1.00 | 25.24 | O |
| ATOM | 1928 | CB | MET | A | 277 | 4.771 | 8.333 | 1.879 | 1.00 | 24.94 | C |
| ATOM | 1929 | CG | MET | A | 277 | 3.996 | 9.631 | 1.753 | 1.00 | 24.31 | C |
| ATOM | 1930 | SD | MET | A | 277 | 5.040 | 11.099 | 2.009 | 1.00 | 25.21 | S |
| ATOM | 1931 | CE | MET | A | 277 | 4.133 | 12.291 | 1.083 | 1.00 | 25.13 | C |
| ATOM | 1932 | N | ALA | A | 278 | 4.910 | 5.239 | 2.829 | 1.00 | 25.57 | N |
| ATOM | 1933 | CA | ALA | A | 278 | 5.694 | 4.033 | 3.067 | 1.00 | 25.99 | C |
| ATOM | 1934 | C | ALA | A | 278 | 5.179 | 2.838 | 2.265 | 1.00 | 26.79 | C |
| ATOM | 1935 | O | ALA | A | 278 | 5.951 | 1.934 | 1.947 | 1.00 | 26.85 | O |
| ATOM | 1936 | CB | ALA | A | 278 | 5.742 | 3.706 | 4.545 | 1.00 | 25.47 | C |
| ATOM | 1937 | N | ARG | A | 279 | 3.884 | 2.843 | 1.941 | 1.00 | 27.59 | N |
| ATOM | 1938 | CA | ARG | A | 279 | 3.272 | 1.799 | 1.111 | 1.00 | 28.44 | C |
| ATOM | 1939 | C | ARG | A | 279 | 3.629 | 1.943 | -0.368 | 1.00 | 28.80 | C |
| ATOM | 1940 | O | ARG | A | 279 | 3.400 | 1.019 | -1.153 | 1.00 | 29.24 | O |
| ATOM | 1941 | CB | ARG | A | 279 | 1.746 | 1.769 | 1.272 | 1.00 | 28.76 | C |
| ATOM | 1942 | CG | ARG | A | 279 | 1.252 | 1.473 | 2.687 | 1.00 | 29.96 | C |
| ATOM | 1943 | CD | ARG | A | 279 | -0.248 | 1.207 | 2.804 | 1.00 | 31.28 | C |
| ATOM | 1944 | NE | ARG | A | 279 | -1.066 | 2.265 | 2.211 | 1.00 | 34.42 | N |
| ATOM | 1945 | CZ | ARG | A | 279 | -1.756 | 3.187 | 2.898 | 1.00 | 35.78 | C |
| ATOM | 1946 | NH1 | ARG | A | 279 | -1.732 | 3.212 | 4.226 | 1.00 | 34.45 | N |
| ATOM | 1947 | NH2 | ARG | A | 279 | -2.475 | 4.096 | 2.242 | 1.00 | 36.50 | N |
| ATOM | 1948 | N | ASP | A | 280 | 4.182 | 3.099 | -0.739 | 1.00 | 29.28 | N |
| ATOM | 1949 | CA | ASP | A | 280 | 4.622 | 3.365 | -2.114 | 1.00 | 29.54 | C |
| ATOM | 1950 | C | ASP | A | 280 | 5.878 | 4.253 | -2.119 | 1.00 | 29.35 | C |
| ATOM | 1951 | O | ASP | A | 280 | 5.847 | 5.391 | -2.592 | 1.00 | 29.52 | O |
| ATOM | 1952 | CB | ASP | A | 280 | 3.481 | 4.016 | -2.907 | 1.00 | 29.96 | C |
| ATOM | 1953 | CG | ASP | A | 280 | 3.700 | 3.981 | -4.416 | 1.00 | 30.61 | C |
| ATOM | 1954 | OD1 | ASP | A | 280 | 4.746 | 3.480 | -4.894 | 1.00 | 30.49 | O |
| ATOM | 1955 | OD2 | ASP | A | 280 | 2.856 | 4.450 | -5.207 | 1.00 | 32.11 | O |
| ATOM | 1956 | N | PRO | A | 281 | 6.989 | 3.711 | -1.617 | 1.00 | 29.24 | N |
| ATOM | 1957 | CA | PRO | A | 281 | 8.175 | 4.509 | -1.297 | 1.00 | 29.16 | C |
| ATOM | 1958 | C | PRO | A | 281 | 8.817 | 5.190 | -2.492 | 1.00 | 29.07 | C |
| ATOM | 1959 | O | PRO | A | 281 | 9.286 | 6.323 | -2.366 | 1.00 | 28.00 | O |
| ATOM | 1960 | CB | PRO | A | 281 | 9.148 | 3.477 | -0.716 | 1.00 | 29.37 | C |
| ATOM | 1961 | CG | PRO | A | 281 | 8.337 | 2.280 | -0.416 | 1.00 | 29.42 | C |
| ATOM | 1962 | CD | PRO | A | 281 | 7.204 | 2.279 | -1.354 | 1.00 | 29.24 | C |
| ATOM | 1963 | N | GLN | A | 282 | 8.843 | 4.493 | -3.625 | 1.00 | 29.78 | N |
| ATOM | 1964 | CA | GLN | A | 282 | 9.511 | 4.974 | -4.834 | 1.00 | 29.92 | C |
| ATOM | 1965 | C | GLN | A | 282 | 8.811 | 6.179 | -5.466 | 1.00 | 29.29 | C |
| ATOM | 1966 | O | GLN | A | 282 | 9.434 | 6.936 | -6.197 | 1.00 | 28.92 | O |
| ATOM | 1967 | CB | GLN | A | 282 | 9.659 | 3.837 | -5.849 | 1.00 | 30.56 | C |
| ATOM | 1968 | CG | GLN | A | 282 | 11.059 | 3.235 | -5.900 | 1.00 | 31.99 | C |
| ATOM | 1969 | CD | GLN | A | 282 | 11.053 | 1.715 | -6.003 | 1.00 | 34.14 | C |
| ATOM | 1970 | OE1 | GLN | A | 282 | 11.116 | 1.164 | -7.102 | 1.00 | 35.63 | O |
| ATOM | 1971 | NE2 | GLN | A | 282 | 10.987 | 1.036 | -4.860 | 1.00 | 34.80 | N |
| ATOM | 1972 | N | ARG | A | 283 | 7.525 | 6.356 | -5.168 | 1.00 | 29.25 | N |
| ATOM | 1973 | CA | ARG | A | 283 | 6.763 | 7.507 | -5.662 | 1.00 | 29.58 | C |
| ATOM | 1974 | C | ARG | A | 283 | 7.077 | 8.807 | -4.909 | 1.00 | 28.96 | C |

FIG. 5GG

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1975 | O | ARG | A | 283 | 7.076 | 9.881 | -5.509 | 1.00 | 29.15 | O |
| ATOM | 1976 | CB | ARG | A | 283 | 5.258 | 7.230 | -5.606 | 1.00 | 29.98 | C |
| ATOM | 1977 | CG | ARG | A | 283 | 4.430 | 8.195 | -6.444 | 1.00 | 32.26 | C |
| ATOM | 1978 | CD | ARG | A | 283 | 3.384 | 8.975 | -5.660 | 1.00 | 34.13 | C |
| ATOM | 1979 | NE | ARG | A | 283 | 3.796 | 10.356 | -5.409 | 1.00 | 35.93 | N |
| ATOM | 1980 | CZ | ARG | A | 283 | 2.967 | 11.396 | -5.359 | 1.00 | 36.56 | C |
| ATOM | 1981 | NH1 | ARG | A | 283 | 1.670 | 11.239 | -5.556 | 1.00 | 36.76 | N |
| ATOM | 1982 | NH2 | ARG | A | 283 | 3.437 | 12.607 | -5.106 | 1.00 | 37.04 | N |
| ATOM | 1983 | N | TYR | A | 284 | 7.344 | 8.702 | -3.606 | 1.00 | 27.79 | N |
| ATOM | 1984 | CA | TYR | A | 284 | 7.514 | 9.875 | -2.749 | 1.00 | 27.02 | C |
| ATOM | 1985 | C | TYR | A | 284 | 8.971 | 10.266 | -2.482 | 1.00 | 26.98 | C |
| ATOM | 1986 | O | TYR | A | 284 | 9.260 | 11.419 | -2.142 | 1.00 | 26.11 | O |
| ATOM | 1987 | CB | TYR | A | 284 | 6.758 | 9.671 | -1.440 | 1.00 | 26.57 | C |
| ATOM | 1988 | CG | TYR | A | 284 | 5.270 | 9.556 | -1.656 | 1.00 | 25.92 | C |
| ATOM | 1989 | CD1 | TYR | A | 284 | 4.636 | 8.310 | -1.667 | 1.00 | 24.81 | C |
| ATOM | 1990 | CE1 | TYR | A | 284 | 3.262 | 8.215 | -1.884 | 1.00 | 25.01 | C |
| ATOM | 1991 | CZ | TYR | A | 284 | 2.520 | 9.372 | -2.101 | 1.00 | 24.76 | C |
| ATOM | 1992 | OH | TYR | A | 284 | 1.159 | 9.308 | -2.310 | 1.00 | 25.67 | O |
| ATOM | 1993 | CE2 | TYR | A | 284 | 3.133 | 10.603 | -2.099 | 1.00 | 24.30 | C |
| ATOM | 1994 | CD2 | TYR | A | 284 | 4.498 | 10.691 | -1.886 | 1.00 | 24.65 | C |
| ATOM | 1995 | N | LEU | A | 285 | 9.876 | 9.302 | -2.628 | 1.00 | 26.74 | N |
| ATOM | 1996 | CA | LEU | A | 285 | 11.307 | 9.567 | -2.515 | 1.00 | 27.31 | C |
| ATOM | 1997 | C | LEU | A | 285 | 12.023 | 9.088 | -3.774 | 1.00 | 27.61 | C |
| ATOM | 1998 | O | LEU | A | 285 | 11.777 | 7.976 | -4.250 | 1.00 | 27.39 | O |
| ATOM | 1999 | CB | LEU | A | 285 | 11.892 | 8.893 | -1.270 | 1.00 | 26.80 | C |
| ATOM | 2000 | CG | LEU | A | 285 | 11.533 | 9.451 | 0.113 | 1.00 | 26.75 | C |
| ATOM | 2001 | CD1 | LEU | A | 285 | 12.421 | 8.819 | 1.176 | 1.00 | 26.78 | C |
| ATOM | 2002 | CD2 | LEU | A | 285 | 11.627 | 10.978 | 0.181 | 1.00 | 25.02 | C |
| ATOM | 2003 | N | VAL | A | 286 | 12.896 | 9.934 | -4.310 | 1.00 | 28.04 | N |
| ATOM | 2004 | CA | VAL | A | 286 | 13.595 | 9.620 | -5.549 | 1.00 | 29.26 | C |
| ATOM | 2005 | C | VAL | A | 286 | 15.069 | 9.306 | -5.299 | 1.00 | 30.07 | C |
| ATOM | 2006 | O | VAL | A | 286 | 15.892 | 10.204 | -5.082 | 1.00 | 30.22 | O |
| ATOM | 2007 | CB | VAL | A | 286 | 13.420 | 10.736 | -6.613 | 1.00 | 29.27 | C |
| ATOM | 2008 | CG1 | VAL | A | 286 | 14.239 | 10.434 | -7.857 | 1.00 | 28.88 | C |
| ATOM | 2009 | CG2 | VAL | A | 286 | 11.951 | 10.894 | -6.976 | 1.00 | 29.23 | C |
| ATOM | 2010 | N | ILE | A | 287 | 15.384 | 8.016 | -5.325 | 1.00 | 30.87 | N |
| ATOM | 2011 | CA | ILE | A | 287 | 16.755 | 7.548 | -5.133 | 1.00 | 31.43 | C |
| ATOM | 2012 | C | ILE | A | 287 | 17.191 | 6.719 | -6.343 | 1.00 | 31.78 | C |
| ATOM | 2013 | O | ILE | A | 287 | 16.435 | 5.870 | -6.823 | 1.00 | 31.94 | O |
| ATOM | 2014 | CB | ILE | A | 287 | 16.884 | 6.749 | -3.807 | 1.00 | 31.42 | C |
| ATOM | 2015 | CG1 | ILE | A | 287 | 16.253 | 7.541 | -2.649 | 1.00 | 30.94 | C |
| ATOM | 2016 | CD1 | ILE | A | 287 | 16.107 | 6.775 | -1.365 | 1.00 | 29.79 | C |
| ATOM | 2017 | CG2 | ILE | A | 287 | 18.353 | 6.431 | -3.505 | 1.00 | 31.01 | C |
| ATOM | 2018 | N | GLN | A | 288 | 18.408 | 6.983 | -6.819 | 1.00 | 32.08 | N |
| ATOM | 2019 | CA | GLN | A | 288 | 18.957 | 6.392 | -8.051 | 1.00 | 32.44 | C |
| ATOM | 2020 | C | GLN | A | 288 | 18.962 | 4.859 | -8.093 | 1.00 | 32.12 | C |
| ATOM | 2021 | O | GLN | A | 288 | 19.237 | 4.188 | -7.097 | 1.00 | 32.37 | O |
| ATOM | 2022 | CB | GLN | A | 288 | 20.373 | 6.931 | -8.316 | 1.00 | 31.90 | C |
| TER | 2023 | | GLN | A | 288 | | | | | | |
| ATOM | 2024 | N | LEU | B | 9 | 35.809 | -0.280 | 55.500 | 1.00 | 36.51 | N |
| ATOM | 2025 | CA | LEU | B | 9 | 35.250 | -0.239 | 54.114 | 1.00 | 36.16 | C |
| ATOM | 2026 | C | LEU | B | 9 | 33.732 | -0.044 | 54.098 | 1.00 | 36.07 | C |
| ATOM | 2027 | O | LEU | B | 9 | 33.007 | -0.581 | 54.941 | 1.00 | 35.35 | O |
| ATOM | 2028 | CB | LEU | B | 9 | 35.628 | -1.501 | 53.337 | 1.00 | 36.62 | C |
| ATOM | 2029 | N | LEU | B | 10 | 33.273 | 0.715 | 53.107 | 1.00 | 36.08 | N |
| ATOM | 2030 | CA | LEU | B | 10 | 31.879 | 1.117 | 52.984 | 1.00 | 35.93 | C |
| ATOM | 2031 | C | LEU | B | 10 | 31.140 | 0.283 | 51.947 | 1.00 | 36.33 | C |
| ATOM | 2032 | O | LEU | B | 10 | 31.656 | 0.005 | 50.864 | 1.00 | 36.38 | O |
| ATOM | 2033 | CB | LEU | B | 10 | 31.811 | 2.599 | 52.609 | 1.00 | 35.82 | C |
| ATOM | 2034 | CG | LEU | B | 10 | 30.467 | 3.253 | 52.289 | 1.00 | 35.50 | C |

FIG. 5HH

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2035 | CD1 | LEU | B | 10 | 29.675 | 3.532 | 53.564 | 1.00 | 35.76 | C |
| ATOM | 2036 | CD2 | LEU | B | 10 | 30.701 | 4.528 | 51.499 | 1.00 | 34.70 | C |
| ATOM | 2037 | N | ARG | B | 11 | 29.919 | -0.108 | 52.287 | 1.00 | 36.51 | N |
| ATOM | 2038 | CA | ARG | B | 11 | 29.059 | -0.811 | 51.351 | 1.00 | 36.75 | C |
| ATOM | 2039 | C | ARG | B | 11 | 27.953 | 0.131 | 50.896 | 1.00 | 36.14 | C |
| ATOM | 2040 | O | ARG | B | 11 | 27.163 | 0.603 | 51.708 | 1.00 | 36.07 | O |
| ATOM | 2041 | CB | ARG | B | 11 | 28.467 | -2.073 | 51.992 | 1.00 | 37.08 | C |
| ATOM | 2042 | CG | ARG | B | 11 | 29.452 | -2.903 | 52.795 | 1.00 | 38.59 | C |
| ATOM | 2043 | CD | ARG | B | 11 | 28.870 | -4.190 | 53.348 | 1.00 | 41.84 | C |
| ATOM | 2044 | NE | ARG | B | 11 | 29.877 | -5.244 | 53.464 | 1.00 | 44.46 | N |
| ATOM | 2045 | CZ | ARG | B | 11 | 29.658 | -6.537 | 53.223 | 1.00 | 46.07 | C |
| ATOM | 2046 | NH1 | ARG | B | 11 | 28.456 | -6.961 | 52.843 | 1.00 | 46.10 | N |
| ATOM | 2047 | NH2 | ARG | B | 11 | 30.649 | -7.412 | 53.360 | 1.00 | 46.50 | N |
| ATOM | 2048 | N | ILE | B | 12 | 27.922 | 0.430 | 49.602 | 1.00 | 35.95 | N |
| ATOM | 2049 | CA | ILE | B | 12 | 26.826 | 1.201 | 49.036 | 1.00 | 35.61 | C |
| ATOM | 2050 | C | ILE | B | 12 | 25.685 | 0.231 | 48.791 | 1.00 | 35.35 | C |
| ATOM | 2051 | O | ILE | B | 12 | 25.714 | -0.538 | 47.836 | 1.00 | 36.12 | O |
| ATOM | 2052 | CB | ILE | B | 12 | 27.246 | 1.940 | 47.743 | 1.00 | 35.75 | C |
| ATOM | 2053 | CG1 | ILE | B | 12 | 28.487 | 2.803 | 47.995 | 1.00 | 36.13 | C |
| ATOM | 2054 | CD1 | ILE | B | 12 | 29.037 | 3.479 | 46.741 | 1.00 | 38.25 | C |
| ATOM | 2055 | CG2 | ILE | B | 12 | 26.094 | 2.809 | 47.223 | 1.00 | 35.27 | C |
| ATOM | 2056 | N | LEU | B | 13 | 24.692 | 0.278 | 49.677 | 1.00 | 34.69 | N |
| ATOM | 2057 | CA | LEU | B | 13 | 23.610 | -0.701 | 49.741 | 1.00 | 33.89 | C |
| ATOM | 2058 | C | LEU | B | 13 | 22.453 | -0.394 | 48.790 | 1.00 | 33.60 | C |
| ATOM | 2059 | O | LEU | B | 13 | 22.276 | 0.743 | 48.354 | 1.00 | 33.47 | O |
| ATOM | 2060 | CB | LEU | B | 13 | 23.077 | -0.775 | 51.179 | 1.00 | 33.85 | C |
| ATOM | 2061 | CG | LEU | B | 13 | 23.550 | -1.878 | 52.134 | 1.00 | 33.47 | C |
| ATOM | 2062 | CD1 | LEU | B | 13 | 25.057 | -1.965 | 52.215 | 1.00 | 31.89 | C |
| ATOM | 2063 | CD2 | LEU | B | 13 | 22.967 | -1.656 | 53.522 | 1.00 | 32.68 | C |
| ATOM | 2064 | N | LYS | B | 14 | 21.668 | -1.427 | 48.497 | 1.00 | 33.25 | N |
| ATOM | 2065 | CA | LYS | B | 14 | 20.450 | -1.323 | 47.696 | 1.00 | 32.95 | C |
| ATOM | 2066 | C | LYS | B | 14 | 19.238 | -1.477 | 48.624 | 1.00 | 32.91 | C |
| ATOM | 2067 | O | LYS | B | 14 | 19.256 | -2.299 | 49.545 | 1.00 | 32.35 | O |
| ATOM | 2068 | CB | LYS | B | 14 | 20.464 | -2.429 | 46.639 | 1.00 | 33.21 | C |
| ATOM | 2069 | CG | LYS | B | 14 | 19.397 | -2.350 | 45.580 | 1.00 | 32.70 | C |
| ATOM | 2070 | CD | LYS | B | 14 | 19.748 | -3.275 | 44.422 | 1.00 | 33.95 | C |
| ATOM | 2071 | CE | LYS | B | 14 | 18.985 | -4.589 | 44.473 | 1.00 | 33.74 | C |
| ATOM | 2072 | NZ | LYS | B | 14 | 18.828 | -5.165 | 43.115 | 1.00 | 34.37 | N |
| ATOM | 2073 | N | GLU | B | 15 | 18.181 | -0.702 | 48.373 | 1.00 | 32.75 | N |
| ATOM | 2074 | CA | GLU | B | 15 | 17.049 | -0.613 | 49.310 | 1.00 | 32.78 | C |
| ATOM | 2075 | C | GLU | B | 15 | 16.366 | -1.930 | 49.675 | 1.00 | 32.45 | C |
| ATOM | 2076 | O | GLU | B | 15 | 15.819 | -2.058 | 50.766 | 1.00 | 32.62 | O |
| ATOM | 2077 | CB | GLU | B | 15 | 16.016 | 0.424 | 48.852 | 1.00 | 32.78 | C |
| ATOM | 2078 | CG | GLU | B | 15 | 15.217 | 0.045 | 47.614 | 1.00 | 33.77 | C |
| ATOM | 2079 | CD | GLU | B | 15 | 14.304 | 1.162 | 47.147 | 1.00 | 34.04 | C |
| ATOM | 2080 | OE1 | GLU | B | 15 | 14.271 | 2.215 | 47.812 | 1.00 | 34.14 | O |
| ATOM | 2081 | OE2 | GLU | B | 15 | 13.615 | 0.983 | 46.117 | 1.00 | 35.01 | O |
| ATOM | 2082 | N | THR | B | 16 | 16.412 | -2.906 | 48.775 | 1.00 | 32.21 | N |
| ATOM | 2083 | CA | THR | B | 16 | 15.783 | -4.206 | 49.009 | 1.00 | 32.16 | C |
| ATOM | 2084 | C | THR | B | 16 | 16.674 | -5.170 | 49.805 | 1.00 | 32.09 | C |
| ATOM | 2085 | O | THR | B | 16 | 16.320 | -6.336 | 49.997 | 1.00 | 32.44 | O |
| ATOM | 2086 | CB | THR | B | 16 | 15.371 | -4.852 | 47.667 | 1.00 | 32.32 | C |
| ATOM | 2087 | OG1 | THR | B | 16 | 16.395 | -4.622 | 46.688 | 1.00 | 32.60 | O |
| ATOM | 2088 | CG2 | THR | B | 16 | 14.151 | -4.147 | 47.078 | 1.00 | 31.88 | C |
| ATOM | 2089 | N | GLU | B | 17 | 17.824 | -4.687 | 50.265 | 1.00 | 31.84 | N |
| ATOM | 2090 | CA | GLU | B | 17 | 18.741 | -5.514 | 51.047 | 1.00 | 32.14 | C |
| ATOM | 2091 | C | GLU | B | 17 | 18.494 | -5.362 | 52.550 | 1.00 | 31.88 | C |
| ATOM | 2092 | O | GLU | B | 17 | 18.961 | -6.177 | 53.346 | 1.00 | 31.76 | O |
| ATOM | 2093 | CB | GLU | B | 17 | 20.198 | -5.193 | 50.702 | 1.00 | 32.22 | C |
| ATOM | 2094 | CG | GLU | B | 17 | 20.569 | -5.477 | 49.256 | 1.00 | 33.17 | C |

FIG. 5II

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2095 | CD | GLU | B | 17 | 22.047 | -5.273 | 48.975 | 1.00 | 35.12 | C |
| ATOM | 2096 | OE1 | GLU | B | 17 | 22.477 | -4.110 | 48.802 | 1.00 | 34.59 | O |
| ATOM | 2097 | OE2 | GLU | B | 17 | 22.783 | -6.282 | 48.917 | 1.00 | 36.62 | O |
| ATOM | 2098 | N | PHE | B | 18 | 17.753 | -4.321 | 52.928 | 1.00 | 31.36 | N |
| ATOM | 2099 | CA | PHE | B | 18 | 17.422 | -4.080 | 54.329 | 1.00 | 31.02 | C |
| ATOM | 2100 | C | PHE | B | 18 | 15.933 | -3.776 | 54.548 | 1.00 | 31.04 | C |
| ATOM | 2101 | O | PHE | B | 18 | 15.230 | -3.359 | 53.627 | 1.00 | 30.91 | O |
| ATOM | 2102 | CB | PHE | B | 18 | 18.319 | -2.982 | 54.935 | 1.00 | 30.55 | C |
| ATOM | 2103 | CG | PHE | B | 18 | 18.177 | -1.626 | 54.280 | 1.00 | 29.89 | C |
| ATOM | 2104 | CD1 | PHE | B | 18 | 17.259 | -0.698 | 54.760 | 1.00 | 29.27 | C |
| ATOM | 2105 | CE1 | PHE | B | 18 | 17.130 | 0.558 | 54.166 | 1.00 | 28.49 | C |
| ATOM | 2106 | CZ | PHE | B | 18 | 17.925 | 0.897 | 53.082 | 1.00 | 28.29 | C |
| ATOM | 2107 | CE2 | PHE | B | 18 | 18.850 | -0.019 | 52.590 | 1.00 | 28.52 | C |
| ATOM | 2108 | CD2 | PHE | B | 18 | 18.982 | -1.269 | 53.196 | 1.00 | 29.36 | C |
| ATOM | 2109 | N | LYS | B | 19 | 15.470 | -3.987 | 55.777 | 1.00 | 30.75 | N |
| ATOM | 2110 | CA | LYS | B | 19 | 14.080 | -3.743 | 56.135 | 1.00 | 30.90 | C |
| ATOM | 2111 | C | LYS | B | 19 | 13.947 | -3.119 | 57.522 | 1.00 | 30.85 | C |
| ATOM | 2112 | O | LYS | B | 19 | 14.409 | -3.687 | 58.513 | 1.00 | 30.82 | O |
| ATOM | 2113 | CB | LYS | B | 19 | 13.272 | -5.046 | 56.077 | 1.00 | 30.67 | C |
| ATOM | 2114 | N | LYS | B | 20 | 13.304 | -1.956 | 57.575 | 1.00 | 30.91 | N |
| ATOM | 2115 | CA | LYS | B | 20 | 12.921 | -1.325 | 58.835 | 1.00 | 31.54 | C |
| ATOM | 2116 | C | LYS | B | 20 | 11.773 | -2.098 | 59.468 | 1.00 | 31.91 | C |
| ATOM | 2117 | O | LYS | B | 20 | 10.773 | -2.394 | 58.804 | 1.00 | 32.29 | O |
| ATOM | 2118 | CB | LYS | B | 20 | 12.471 | 0.121 | 58.608 | 1.00 | 31.68 | C |
| ATOM | 2119 | CG | LYS | B | 20 | 13.489 | 1.027 | 57.960 | 1.00 | 32.01 | C |
| ATOM | 2120 | CD | LYS | B | 20 | 12.827 | 2.338 | 57.566 | 1.00 | 33.94 | C |
| ATOM | 2121 | CE | LYS | B | 20 | 13.007 | 2.631 | 56.091 | 1.00 | 35.02 | C |
| ATOM | 2122 | NZ | LYS | B | 20 | 13.598 | 3.988 | 55.903 | 1.00 | 36.81 | N |
| ATOM | 2123 | N | ILE | B | 21 | 11.913 | -2.411 | 60.752 | 1.00 | 32.24 | N |
| ATOM | 2124 | CA | ILE | B | 21 | 10.881 | -3.133 | 61.484 | 1.00 | 32.61 | C |
| ATOM | 2125 | C | ILE | B | 21 | 10.252 | -2.287 | 62.606 | 1.00 | 33.07 | C |
| ATOM | 2126 | O | ILE | B | 21 | 9.038 | -2.302 | 62.780 | 1.00 | 33.91 | O |
| ATOM | 2127 | CB | ILE | B | 21 | 11.421 | -4.513 | 61.982 | 1.00 | 32.64 | C |
| ATOM | 2128 | CG1 | ILE | B | 21 | 11.042 | -5.615 | 60.991 | 1.00 | 32.36 | C |
| ATOM | 2129 | CD1 | ILE | B | 21 | 12.190 | -6.499 | 60.574 | 1.00 | 32.32 | C |
| ATOM | 2130 | CG2 | ILE | B | 21 | 10.888 | -4.874 | 63.362 | 1.00 | 32.84 | C |
| ATOM | 2131 | N | LYS | B | 22 | 11.064 | -1.538 | 63.348 | 1.00 | 33.18 | N |
| ATOM | 2132 | CA | LYS | B | 22 | 10.540 | -0.695 | 64.426 | 1.00 | 33.02 | C |
| ATOM | 2133 | C | LYS | B | 22 | 11.362 | 0.580 | 64.645 | 1.00 | 32.45 | C |
| ATOM | 2134 | O | LYS | B | 22 | 12.582 | 0.582 | 64.466 | 1.00 | 32.37 | O |
| ATOM | 2135 | CB | LYS | B | 22 | 10.378 | -1.511 | 65.722 | 1.00 | 33.28 | C |
| ATOM | 2136 | CG | LYS | B | 22 | 11.252 | -1.096 | 66.895 | 1.00 | 34.72 | C |
| ATOM | 2137 | CD | LYS | B | 22 | 10.965 | -1.947 | 68.134 | 1.00 | 36.26 | C |
| ATOM | 2138 | CE | LYS | B | 22 | 10.344 | -1.116 | 69.265 | 1.00 | 37.38 | C |
| ATOM | 2139 | NZ | LYS | B | 22 | 11.158 | 0.095 | 69.624 | 1.00 | 37.93 | N |
| ATOM | 2140 | N | VAL | B | 23 | 10.672 | 1.658 | 65.016 | 1.00 | 31.81 | N |
| ATOM | 2141 | CA | VAL | B | 23 | 11.295 | 2.947 | 65.312 | 1.00 | 31.31 | C |
| ATOM | 2142 | C | VAL | B | 23 | 11.936 | 2.915 | 66.701 | 1.00 | 31.22 | C |
| ATOM | 2143 | O | VAL | B | 23 | 11.312 | 2.471 | 67.669 | 1.00 | 31.50 | O |
| ATOM | 2144 | CB | VAL | B | 23 | 10.263 | 4.112 | 65.231 | 1.00 | 31.66 | C |
| ATOM | 2145 | CG1 | VAL | B | 23 | 10.937 | 5.466 | 65.411 | 1.00 | 30.71 | C |
| ATOM | 2146 | CG2 | VAL | B | 23 | 9.520 | 4.082 | 63.910 | 1.00 | 30.77 | C |
| ATOM | 2147 | N | LEU | B | 24 | 13.183 | 3.374 | 66.786 | 1.00 | 30.78 | N |
| ATOM | 2148 | CA | LEU | B | 24 | 13.927 | 3.382 | 68.043 | 1.00 | 30.60 | C |
| ATOM | 2149 | C | LEU | B | 24 | 14.085 | 4.781 | 68.614 | 1.00 | 30.65 | C |
| ATOM | 2150 | O | LEU | B | 24 | 14.251 | 4.946 | 69.822 | 1.00 | 30.68 | O |
| ATOM | 2151 | CB | LEU | B | 24 | 15.315 | 2.764 | 67.863 | 1.00 | 30.72 | C |
| ATOM | 2152 | CG | LEU | B | 24 | 15.442 | 1.295 | 67.475 | 1.00 | 30.42 | C |
| ATOM | 2153 | CD1 | LEU | B | 24 | 16.908 | 0.921 | 67.455 | 1.00 | 29.08 | C |
| ATOM | 2154 | CD2 | LEU | B | 24 | 14.646 | 0.377 | 68.422 | 1.00 | 31.11 | C |

FIG. 5JJ

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2155 | N | GLY | B | 25 | 14.044 | 5.784 | 67.746 | 1.00 | 30.59 | N |
| ATOM | 2156 | CA | GLY | B | 25 | 14.208 | 7.155 | 68.179 | 1.00 | 31.08 | C |
| ATOM | 2157 | C | GLY | B | 25 | 14.509 | 8.120 | 67.054 | 1.00 | 31.75 | C |
| ATOM | 2158 | O | GLY | B | 25 | 14.409 | 7.777 | 65.869 | 1.00 | 31.24 | O |
| ATOM | 2159 | N | SER | B | 26 | 14.876 | 9.337 | 67.444 | 1.00 | 32.16 | N |
| ATOM | 2160 | CA | SER | B | 26 | 15.187 | 10.412 | 66.511 | 1.00 | 33.09 | C |
| ATOM | 2161 | C | SER | B | 26 | 16.125 | 11.447 | 67.141 | 1.00 | 33.40 | C |
| ATOM | 2162 | O | SER | B | 26 | 16.416 | 11.392 | 68.336 | 1.00 | 33.11 | O |
| ATOM | 2163 | CB | SER | B | 26 | 13.902 | 11.095 | 66.036 | 1.00 | 32.88 | C |
| ATOM | 2164 | OG | SER | B | 26 | 13.078 | 11.437 | 67.135 | 1.00 | 33.34 | O |
| ATOM | 2165 | N | GLY | B | 27 | 16.594 | 12.377 | 66.315 | 1.00 | 33.88 | N |
| ATOM | 2166 | CA | GLY | B | 27 | 17.429 | 13.480 | 66.748 | 1.00 | 34.41 | C |
| ATOM | 2167 | C | GLY | B | 27 | 17.428 | 14.573 | 65.696 | 1.00 | 35.04 | C |
| ATOM | 2168 | O | GLY | B | 27 | 16.602 | 14.571 | 64.780 | 1.00 | 35.00 | O |
| ATOM | 2169 | N | ALA | B | 28 | 18.362 | 15.510 | 65.825 | 1.00 | 35.78 | N |
| ATOM | 2170 | CA | ALA | B | 28 | 18.546 | 16.561 | 64.827 | 1.00 | 36.05 | C |
| ATOM | 2171 | C | ALA | B | 28 | 18.841 | 16.000 | 63.436 | 1.00 | 36.09 | C |
| ATOM | 2172 | O | ALA | B | 28 | 18.481 | 16.621 | 62.436 | 1.00 | 36.99 | O |
| ATOM | 2173 | CB | ALA | B | 28 | 19.645 | 17.526 | 65.259 | 1.00 | 36.12 | C |
| ATOM | 2174 | N | PHE | B | 29 | 19.471 | 14.826 | 63.369 | 1.00 | 35.99 | N |
| ATOM | 2175 | CA | PHE | B | 29 | 19.887 | 14.256 | 62.079 | 1.00 | 35.68 | C |
| ATOM | 2176 | C | PHE | B | 29 | 18.854 | 13.371 | 61.380 | 1.00 | 34.69 | C |
| ATOM | 2177 | O | PHE | B | 29 | 18.897 | 13.216 | 60.163 | 1.00 | 34.81 | O |
| ATOM | 2178 | CB | PHE | B | 29 | 21.238 | 13.551 | 62.199 | 1.00 | 36.19 | C |
| ATOM | 2179 | CG | PHE | B | 29 | 22.347 | 14.451 | 62.678 | 1.00 | 38.34 | C |
| ATOM | 2180 | CD1 | PHE | B | 29 | 22.659 | 15.627 | 61.993 | 1.00 | 39.30 | C |
| ATOM | 2181 | CE1 | PHE | B | 29 | 23.676 | 16.456 | 62.431 | 1.00 | 39.60 | C |
| ATOM | 2182 | CZ | PHE | B | 29 | 24.398 | 16.122 | 63.573 | 1.00 | 40.23 | C |
| ATOM | 2183 | CE2 | PHE | B | 29 | 24.099 | 14.955 | 64.269 | 1.00 | 39.74 | C |
| ATOM | 2184 | CD2 | PHE | B | 29 | 23.073 | 14.130 | 63.821 | 1.00 | 39.17 | C |
| ATOM | 2185 | N | GLY | B | 30 | 17.937 | 12.784 | 62.143 | 1.00 | 33.88 | N |
| ATOM | 2186 | CA | GLY | B | 30 | 16.847 | 12.017 | 61.567 | 1.00 | 32.69 | C |
| ATOM | 2187 | C | GLY | B | 30 | 16.368 | 10.866 | 62.425 | 1.00 | 31.96 | C |
| ATOM | 2188 | O | GLY | B | 30 | 16.805 | 10.697 | 63.563 | 1.00 | 33.12 | O |
| ATOM | 2189 | N | THR | B | 31 | 15.467 | 10.067 | 61.867 | 1.00 | 30.52 | N |
| ATOM | 2190 | CA | THR | B | 31 | 14.843 | 8.956 | 62.578 | 1.00 | 28.81 | C |
| ATOM | 2191 | C | THR | B | 31 | 15.733 | 7.716 | 62.564 | 1.00 | 28.63 | C |
| ATOM | 2192 | O | THR | B | 31 | 16.400 | 7.430 | 61.568 | 1.00 | 28.17 | O |
| ATOM | 2193 | CB | THR | B | 31 | 13.462 | 8.632 | 61.939 | 1.00 | 28.33 | C |
| ATOM | 2194 | OG1 | THR | B | 31 | 12.636 | 9.799 | 61.982 | 1.00 | 26.97 | O |
| ATOM | 2195 | CG2 | THR | B | 31 | 12.678 | 7.624 | 62.777 | 1.00 | 26.74 | C |
| ATOM | 2196 | N | VAL | B | 32 | 15.723 | 6.984 | 63.677 | 1.00 | 28.10 | N |
| ATOM | 2197 | CA | VAL | B | 32 | 16.490 | 5.753 | 63.805 | 1.00 | 27.94 | C |
| ATOM | 2198 | C | VAL | B | 32 | 15.573 | 4.532 | 63.955 | 1.00 | 27.59 | C |
| ATOM | 2199 | O | VAL | B | 32 | 14.689 | 4.514 | 64.815 | 1.00 | 27.23 | O |
| ATOM | 2200 | CB | VAL | B | 32 | 17.477 | 5.808 | 64.995 | 1.00 | 27.56 | C |
| ATOM | 2201 | CG1 | VAL | B | 32 | 18.536 | 4.730 | 64.845 | 1.00 | 27.73 | C |
| ATOM | 2202 | CG2 | VAL | B | 32 | 18.123 | 7.182 | 65.106 | 1.00 | 28.46 | C |
| ATOM | 2203 | N | TYR | B | 33 | 15.813 | 3.515 | 63.126 | 1.00 | 26.88 | N |
| ATOM | 2204 | CA | TYR | B | 33 | 15.003 | 2.299 | 63.109 | 1.00 | 26.99 | C |
| ATOM | 2205 | C | TYR | B | 33 | 15.814 | 1.074 | 63.494 | 1.00 | 27.45 | C |
| ATOM | 2206 | O | TYR | B | 33 | 17.009 | 0.988 | 63.196 | 1.00 | 27.54 | O |
| ATOM | 2207 | CB | TYR | B | 33 | 14.430 | 2.043 | 61.711 | 1.00 | 26.40 | C |
| ATOM | 2208 | CG | TYR | B | 33 | 13.471 | 3.082 | 61.204 | 1.00 | 25.33 | C |
| ATOM | 2209 | CD1 | TYR | B | 33 | 12.089 | 2.879 | 61.286 | 1.00 | 24.58 | C |
| ATOM | 2210 | CE1 | TYR | B | 33 | 11.201 | 3.829 | 60.813 | 1.00 | 23.85 | C |
| ATOM | 2211 | CZ | TYR | B | 33 | 11.687 | 4.992 | 60.242 | 1.00 | 23.71 | C |
| ATOM | 2212 | OH | TYR | B | 33 | 10.811 | 5.926 | 59.777 | 1.00 | 25.43 | O |
| ATOM | 2213 | CE2 | TYR | B | 33 | 13.046 | 5.221 | 60.134 | 1.00 | 23.94 | C |
| ATOM | 2214 | CD2 | TYR | B | 33 | 13.936 | 4.262 | 60.616 | 1.00 | 24.69 | C |

FIG. 5KK

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|---------|--------|------|-------|---|
| ATOM | 2215 | N | LYS | B | 34 | 15.154 | 0.130 | 64.155 | 1.00 | 27.60 | N |
| ATOM | 2216 | CA | LYS | B | 34 | 15.668 | -1.224 | 64.241 | 1.00 | 28.46 | C |
| ATOM | 2217 | C | LYS | B | 34 | 15.188 | -1.958 | 62.994 | 1.00 | 28.86 | C |
| ATOM | 2218 | O | LYS | B | 34 | 14.002 | -1.898 | 62.628 | 1.00 | 29.23 | O |
| ATOM | 2219 | CB | LYS | B | 34 | 15.212 | -1.923 | 65.528 | 1.00 | 28.56 | C |
| ATOM | 2220 | CG | LYS | B | 34 | 14.487 | -3.259 | 65.338 | 1.00 | 29.67 | C |
| ATOM | 2221 | CD | LYS | B | 34 | 15.401 | -4.453 | 65.615 | 1.00 | 30.39 | C |
| ATOM | 2222 | CE | LYS | B | 34 | 15.319 | -4.864 | 67.081 | 1.00 | 30.86 | C |
| ATOM | 2223 | NZ | LYS | B | 34 | 15.267 | -6.344 | 67.236 | 1.00 | 31.69 | N |
| ATOM | 2224 | N | GLY | B | 35 | 16.121 | -2.625 | 62.330 | 1.00 | 28.88 | N |
| ATOM | 2225 | CA | GLY | B | 35 | 15.803 | -3.350 | 61.120 | 1.00 | 29.29 | C |
| ATOM | 2226 | C | GLY | B | 35 | 16.651 | -4.580 | 60.893 | 1.00 | 29.43 | C |
| ATOM | 2227 | O | GLY | B | 35 | 17.472 | -4.963 | 61.738 | 1.00 | 28.80 | O |
| ATOM | 2228 | N | LEU | B | 36 | 16.434 | -5.202 | 59.738 | 1.00 | 29.90 | N |
| ATOM | 2229 | CA | LEU | B | 36 | 17.175 | -6.393 | 59.346 | 1.00 | 30.45 | C |
| ATOM | 2230 | C | LEU | B | 36 | 17.904 | -6.144 | 58.037 | 1.00 | 31.07 | C |
| ATOM | 2231 | O | LEU | B | 36 | 17.440 | -5.373 | 57.200 | 1.00 | 31.12 | O |
| ATOM | 2232 | CB | LEU | B | 36 | 16.235 | -7.594 | 59.217 | 1.00 | 30.34 | C |
| ATOM | 2233 | CG | LEU | B | 36 | 15.604 | -8.171 | 60.494 | 1.00 | 30.19 | C |
| ATOM | 2234 | CD1 | LEU | B | 36 | 14.686 | -9.355 | 60.158 | 1.00 | 29.69 | C |
| ATOM | 2235 | CD2 | LEU | B | 36 | 16.664 | -8.589 | 61.508 | 1.00 | 29.41 | C |
| ATOM | 2236 | N | TRP | B | 37 | 19.051 | -6.796 | 57.876 | 1.00 | 32.05 | N |
| ATOM | 2237 | CA | TRP | B | 37 | 19.906 | -6.622 | 56.706 | 1.00 | 32.98 | C |
| ATOM | 2238 | C | TRP | B | 37 | 20.497 | -7.963 | 56.241 | 1.00 | 33.39 | C |
| ATOM | 2239 | O | TRP | B | 37 | 21.000 | -8.745 | 57.053 | 1.00 | 32.84 | O |
| ATOM | 2240 | CB | TRP | B | 37 | 21.021 | -5.619 | 57.033 | 1.00 | 33.12 | C |
| ATOM | 2241 | CG | TRP | B | 37 | 22.147 | -5.537 | 56.037 | 1.00 | 34.77 | C |
| ATOM | 2242 | CD1 | TRP | B | 37 | 22.048 | -5.546 | 54.670 | 1.00 | 35.24 | C |
| ATOM | 2243 | NE1 | TRP | B | 37 | 23.295 | -5.441 | 54.104 | 1.00 | 36.21 | N |
| ATOM | 2244 | CE2 | TRP | B | 37 | 24.234 | -5.357 | 55.099 | 1.00 | 36.82 | C |
| ATOM | 2245 | CD2 | TRP | B | 37 | 23.545 | -5.410 | 56.333 | 1.00 | 36.13 | C |
| ATOM | 2246 | CE3 | TRP | B | 37 | 24.290 | -5.333 | 57.522 | 1.00 | 36.03 | C |
| ATOM | 2247 | CZ3 | TRP | B | 37 | 25.675 | -5.213 | 57.443 | 1.00 | 37.00 | C |
| ATOM | 2248 | CH2 | TRP | B | 37 | 26.331 | -5.163 | 56.198 | 1.00 | 37.38 | C |
| ATOM | 2249 | CZ2 | TRP | B | 37 | 25.631 | -5.237 | 55.018 | 1.00 | 37.67 | C |
| ATOM | 2250 | N | ILE | B | 38 | 20.423 | -8.213 | 54.935 | 1.00 | 34.01 | N |
| ATOM | 2251 | CA | ILE | B | 38 | 21.105 | -9.349 | 54.313 | 1.00 | 34.78 | C |
| ATOM | 2252 | C | ILE | B | 38 | 22.273 | -8.852 | 53.448 | 1.00 | 35.19 | C |
| ATOM | 2253 | O | ILE | B | 38 | 22.061 | -8.332 | 52.350 | 1.00 | 35.24 | O |
| ATOM | 2254 | CB | ILE | B | 38 | 20.124 | -10.209 | 53.481 | 1.00 | 34.91 | C |
| ATOM | 2255 | CG1 | ILE | B | 38 | 18.917 | -10.626 | 54.326 | 1.00 | 34.87 | C |
| ATOM | 2256 | CD1 | ILE | B | 38 | 17.624 | -10.739 | 53.544 | 1.00 | 35.11 | C |
| ATOM | 2257 | CG2 | ILE | B | 38 | 20.833 | -11.450 | 52.924 | 1.00 | 34.63 | C |
| ATOM | 2258 | N | PRO | B | 39 | 23.500 | -9.017 | 53.947 | 1.00 | 35.54 | N |
| ATOM | 2259 | CA | PRO | B | 39 | 24.706 | -8.528 | 53.260 | 1.00 | 35.80 | C |
| ATOM | 2260 | C | PRO | B | 39 | 24.896 | -9.146 | 51.878 | 1.00 | 35.80 | C |
| ATOM | 2261 | O | PRO | B | 39 | 24.442 | -10.272 | 51.668 | 1.00 | 35.94 | O |
| ATOM | 2262 | CB | PRO | B | 39 | 25.846 | -8.979 | 54.183 | 1.00 | 36.00 | C |
| ATOM | 2263 | CG | PRO | B | 39 | 25.206 | -9.208 | 55.512 | 1.00 | 36.08 | C |
| ATOM | 2264 | CD | PRO | B | 39 | 23.827 | -9.706 | 55.209 | 1.00 | 35.61 | C |
| ATOM | 2265 | N | LYS | B | 45 | 19.967 | -12.673 | 58.006 | 1.00 | 30.23 | N |
| ATOM | 2266 | CA | LYS | B | 45 | 19.319 | -11.416 | 58.348 | 1.00 | 29.73 | C |
| ATOM | 2267 | C | LYS | B | 45 | 19.892 | -10.909 | 59.656 | 1.00 | 29.68 | C |
| ATOM | 2268 | O | LYS | B | 45 | 19.529 | -11.385 | 60.738 | 1.00 | 30.40 | O |
| ATOM | 2269 | CB | LYS | B | 45 | 17.801 | -11.590 | 58.438 | 1.00 | 29.91 | C |
| ATOM | 2270 | CG | LYS | B | 45 | 17.173 | -12.197 | 57.179 | 1.00 | 29.96 | C |
| ATOM | 2271 | CD | LYS | B | 45 | 15.689 | -12.478 | 57.360 | 1.00 | 29.04 | C |
| ATOM | 2272 | CE | LYS | B | 45 | 15.006 | -12.671 | 56.023 | 1.00 | 28.79 | C |
| ATOM | 2273 | NZ | LYS | B | 45 | 13.514 | -12.655 | 56.141 | 1.00 | 29.30 | N |
| ATOM | 2274 | N | ILE | B | 46 | 20.816 | -9.959 | 59.546 | 1.00 | 29.44 | N |

FIG. 5LL

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|---------|--------|------|-------|---|
| ATOM | 2275 | CA | ILE | B | 46 | 21.479 | -9.376 | 60.706 | 1.00 | 29.19 | C |
| ATOM | 2276 | C | ILE | B | 46 | 20.662 | -8.185 | 61.214 | 1.00 | 28.84 | C |
| ATOM | 2277 | O | ILE | B | 46 | 20.242 | -7.343 | 60.417 | 1.00 | 28.97 | O |
| ATOM | 2278 | CB | ILE | B | 46 | 22.912 | -8.934 | 60.342 | 1.00 | 29.26 | C |
| ATOM | 2279 | CG1 | ILE | B | 46 | 23.760 | -10.133 | 59.905 | 1.00 | 29.53 | C |
| ATOM | 2280 | CD1 | ILE | B | 46 | 25.123 | -9.739 | 59.314 | 1.00 | 30.04 | C |
| ATOM | 2281 | CG2 | ILE | B | 46 | 23.580 | -8.219 | 61.517 | 1.00 | 30.05 | C |
| ATOM | 2282 | N | PRO | B | 47 | 20.406 | -8.130 | 62.524 | 1.00 | 28.40 | N |
| ATOM | 2283 | CA | PRO | B | 47 | 19.812 | -6.934 | 63.139 | 1.00 | 27.73 | C |
| ATOM | 2284 | C | PRO | B | 47 | 20.737 | -5.735 | 62.997 | 1.00 | 27.16 | C |
| ATOM | 2285 | O | PRO | B | 47 | 21.955 | -5.874 | 63.158 | 1.00 | 27.70 | O |
| ATOM | 2286 | CB | PRO | B | 47 | 19.674 | -7.316 | 64.617 | 1.00 | 27.98 | C |
| ATOM | 2287 | CG | PRO | B | 47 | 19.742 | -8.811 | 64.653 | 1.00 | 28.63 | C |
| ATOM | 2288 | CD | PRO | B | 47 | 20.630 | -9.207 | 63.505 | 1.00 | 28.50 | C |
| ATOM | 2289 | N | VAL | B | 48 | 20.165 | -4.573 | 62.691 | 1.00 | 25.96 | N |
| ATOM | 2290 | CA | VAL | B | 48 | 20.945 | -3.345 | 62.529 | 1.00 | 24.24 | C |
| ATOM | 2291 | C | VAL | B | 48 | 20.146 | -2.134 | 62.976 | 1.00 | 23.62 | C |
| ATOM | 2292 | O | VAL | B | 48 | 18.928 | -2.217 | 63.176 | 1.00 | 22.76 | O |
| ATOM | 2293 | CB | VAL | B | 48 | 21.381 | -3.097 | 61.045 | 1.00 | 24.08 | C |
| ATOM | 2294 | CG1 | VAL | B | 48 | 22.525 | -4.026 | 60.627 | 1.00 | 24.06 | C |
| ATOM | 2295 | CG2 | VAL | B | 48 | 20.191 | -3.202 | 60.086 | 1.00 | 23.55 | C |
| ATOM | 2296 | N | ALA | B | 49 | 20.849 | -1.013 | 63.129 | 1.00 | 22.63 | N |
| ATOM | 2297 | CA | ALA | B | 49 | 20.207 | 0.289 | 63.206 | 1.00 | 22.02 | C |
| ATOM | 2298 | C | ALA | B | 49 | 20.155 | 0.861 | 61.800 | 1.00 | 21.80 | C |
| ATOM | 2299 | O | ALA | B | 49 | 21.135 | 0.783 | 61.052 | 1.00 | 21.25 | O |
| ATOM | 2300 | CB | ALA | B | 49 | 20.961 | 1.221 | 64.146 | 1.00 | 20.54 | C |
| ATOM | 2301 | N | ILE | B | 50 | 19.001 | 1.406 | 61.430 | 1.00 | 22.56 | N |
| ATOM | 2302 | CA | ILE | B | 50 | 18.867 | 2.144 | 60.171 | 1.00 | 23.43 | C |
| ATOM | 2303 | C | ILE | B | 50 | 18.496 | 3.581 | 60.505 | 1.00 | 23.73 | C |
| ATOM | 2304 | O | ILE | B | 50 | 17.483 | 3.832 | 61.154 | 1.00 | 23.88 | O |
| ATOM | 2305 | CB | ILE | B | 50 | 17.791 | 1.525 | 59.231 | 1.00 | 23.24 | C |
| ATOM | 2306 | CG1 | ILE | B | 50 | 18.074 | 0.047 | 58.952 | 1.00 | 24.08 | C |
| ATOM | 2307 | CD1 | ILE | B | 50 | 16.870 | -0.718 | 58.352 | 1.00 | 23.64 | C |
| ATOM | 2308 | CG2 | ILE | B | 50 | 17.724 | 2.303 | 57.924 | 1.00 | 23.02 | C |
| ATOM | 2309 | N | LYS | B | 51 | 19.322 | 4.515 | 60.060 | 1.00 | 24.31 | N |
| ATOM | 2310 | CA | LYS | B | 51 | 19.073 | 5.925 | 60.289 | 1.00 | 25.12 | C |
| ATOM | 2311 | C | LYS | B | 51 | 18.703 | 6.613 | 58.987 | 1.00 | 25.12 | C |
| ATOM | 2312 | O | LYS | B | 51 | 19.522 | 6.703 | 58.077 | 1.00 | 25.25 | O |
| ATOM | 2313 | CB | LYS | B | 51 | 20.303 | 6.585 | 60.905 | 1.00 | 25.49 | C |
| ATOM | 2314 | CG | LYS | B | 51 | 20.044 | 7.959 | 61.496 | 1.00 | 26.70 | C |
| ATOM | 2315 | CD | LYS | B | 51 | 21.338 | 8.562 | 62.016 | 1.00 | 29.12 | C |
| ATOM | 2316 | CE | LYS | B | 51 | 21.485 | 8.372 | 63.519 | 1.00 | 30.08 | C |
| ATOM | 2317 | NZ | LYS | B | 51 | 21.591 | 9.691 | 64.199 | 1.00 | 31.87 | N |
| ATOM | 2318 | N | GLU | B | 52 | 17.458 | 7.078 | 58.912 | 1.00 | 25.40 | N |
| ATOM | 2319 | CA | GLU | B | 52 | 16.968 | 7.883 | 57.799 | 1.00 | 25.56 | C |
| ATOM | 2320 | C | GLU | B | 52 | 17.242 | 9.350 | 58.115 | 1.00 | 25.32 | C |
| ATOM | 2321 | O | GLU | B | 52 | 16.732 | 9.886 | 59.102 | 1.00 | 25.38 | O |
| ATOM | 2322 | CB | GLU | B | 52 | 15.469 | 7.646 | 57.579 | 1.00 | 25.71 | C |
| ATOM | 2323 | CG | GLU | B | 52 | 14.950 | 8.046 | 56.199 | 1.00 | 27.70 | C |
| ATOM | 2324 | CD | GLU | B | 52 | 13.672 | 7.303 | 55.805 | 1.00 | 29.86 | C |
| ATOM | 2325 | OE1 | GLU | B | 52 | 13.644 | 6.652 | 54.733 | 1.00 | 30.54 | O |
| ATOM | 2326 | OE2 | GLU | B | 52 | 12.689 | 7.356 | 56.568 | 1.00 | 31.09 | O |
| ATOM | 2327 | N | LEU | B | 53 | 18.052 | 9.991 | 57.278 | 1.00 | 25.08 | N |
| ATOM | 2328 | CA | LEU | B | 53 | 18.479 | 11.360 | 57.524 | 1.00 | 25.43 | C |
| ATOM | 2329 | C | LEU | B | 53 | 17.428 | 12.348 | 57.049 | 1.00 | 25.68 | C |
| ATOM | 2330 | O | LEU | B | 53 | 17.056 | 12.340 | 55.873 | 1.00 | 26.42 | O |
| ATOM | 2331 | CB | LEU | B | 53 | 19.821 | 11.631 | 56.833 | 1.00 | 24.84 | C |
| ATOM | 2332 | CG | LEU | B | 53 | 21.143 | 11.472 | 57.596 | 1.00 | 25.17 | C |
| ATOM | 2333 | CD1 | LEU | B | 53 | 21.104 | 10.390 | 58.687 | 1.00 | 24.31 | C |
| ATOM | 2334 | CD2 | LEU | B | 53 | 22.282 | 11.211 | 56.620 | 1.00 | 23.23 | C |

FIG. 5MM

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2335 | N | LYS | B | 60 | 24.107 | 19.303 | 48.871 | 1.00 | 35.82 | N |
| ATOM | 2336 | CA | LYS | B | 60 | 25.287 | 18.437 | 48.864 | 1.00 | 35.63 | C |
| ATOM | 2337 | C | LYS | B | 60 | 25.186 | 17.305 | 47.836 | 1.00 | 35.36 | C |
| ATOM | 2338 | O | LYS | B | 60 | 24.183 | 16.588 | 47.775 | 1.00 | 35.49 | O |
| ATOM | 2339 | CB | LYS | B | 60 | 25.542 | 17.867 | 50.264 | 1.00 | 35.81 | C |
| ATOM | 2340 | N | ALA | B | 61 | 26.245 | 17.145 | 47.045 | 1.00 | 34.96 | N |
| ATOM | 2341 | CA | ALA | B | 61 | 26.293 | 16.139 | 45.987 | 1.00 | 34.41 | C |
| ATOM | 2342 | C | ALA | B | 61 | 26.533 | 14.721 | 46.519 | 1.00 | 34.23 | C |
| ATOM | 2343 | O | ALA | B | 61 | 27.185 | 14.533 | 47.545 | 1.00 | 33.85 | O |
| ATOM | 2344 | CB | ALA | B | 61 | 27.357 | 16.506 | 44.981 | 1.00 | 33.96 | C |
| ATOM | 2345 | N | ASN | B | 62 | 26.021 | 13.729 | 45.795 | 1.00 | 33.90 | N |
| ATOM | 2346 | CA | ASN | B | 62 | 26.219 | 12.327 | 46.148 | 1.00 | 33.88 | C |
| ATOM | 2347 | C | ASN | B | 62 | 27.690 | 11.941 | 46.261 | 1.00 | 33.85 | C |
| ATOM | 2348 | O | ASN | B | 62 | 28.055 | 11.124 | 47.108 | 1.00 | 33.65 | O |
| ATOM | 2349 | CB | ASN | B | 62 | 25.497 | 11.408 | 45.161 | 1.00 | 33.62 | C |
| ATOM | 2350 | CG | ASN | B | 62 | 23.988 | 11.546 | 45.229 | 1.00 | 33.51 | C |
| ATOM | 2351 | OD1 | ASN | B | 62 | 23.438 | 11.999 | 46.233 | 1.00 | 32.94 | O |
| ATOM | 2352 | ND2 | ASN | B | 62 | 23.308 | 11.156 | 44.153 | 1.00 | 33.25 | N |
| ATOM | 2353 | N | LYS | B | 63 | 28.519 | 12.537 | 45.405 | 1.00 | 34.03 | N |
| ATOM | 2354 | CA | LYS | B | 63 | 29.973 | 12.398 | 45.470 | 1.00 | 34.37 | C |
| ATOM | 2355 | C | LYS | B | 63 | 30.515 | 12.813 | 46.844 | 1.00 | 34.47 | C |
| ATOM | 2356 | O | LYS | B | 63 | 31.297 | 12.083 | 47.462 | 1.00 | 34.54 | O |
| ATOM | 2357 | CB | LYS | B | 63 | 30.630 | 13.228 | 44.364 | 1.00 | 34.22 | C |
| ATOM | 2358 | CG | LYS | B | 63 | 32.119 | 13.443 | 44.550 | 1.00 | 34.56 | C |
| ATOM | 2359 | CD | LYS | B | 63 | 32.742 | 14.126 | 43.350 | 1.00 | 35.60 | C |
| ATOM | 2360 | CE | LYS | B | 63 | 34.118 | 13.554 | 43.056 | 1.00 | 36.59 | C |
| ATOM | 2361 | NZ | LYS | B | 63 | 35.129 | 13.939 | 44.093 | 1.00 | 37.21 | N |
| ATOM | 2362 | N | GLU | B | 64 | 30.084 | 13.982 | 47.312 | 1.00 | 34.76 | N |
| ATOM | 2363 | CA | GLU | B | 64 | 30.470 | 14.490 | 48.623 | 1.00 | 35.26 | C |
| ATOM | 2364 | C | GLU | B | 64 | 30.025 | 13.525 | 49.722 | 1.00 | 34.76 | C |
| ATOM | 2365 | O | GLU | B | 64 | 30.840 | 13.091 | 50.540 | 1.00 | 35.19 | O |
| ATOM | 2366 | CB | GLU | B | 64 | 29.875 | 15.884 | 48.855 | 1.00 | 36.16 | C |
| ATOM | 2367 | CG | GLU | B | 64 | 30.712 | 17.028 | 48.296 | 1.00 | 38.54 | C |
| ATOM | 2368 | CD | GLU | B | 64 | 29.896 | 18.033 | 47.494 | 1.00 | 41.32 | C |
| ATOM | 2369 | OE1 | GLU | B | 64 | 30.210 | 18.236 | 46.299 | 1.00 | 42.74 | O |
| ATOM | 2370 | OE2 | GLU | B | 64 | 28.946 | 18.631 | 48.050 | 1.00 | 42.99 | O |
| ATOM | 2371 | N | ILE | B | 65 | 28.739 | 13.172 | 49.712 | 1.00 | 34.08 | N |
| ATOM | 2372 | CA | ILE | B | 65 | 28.152 | 12.287 | 50.717 | 1.00 | 33.11 | C |
| ATOM | 2373 | C | ILE | B | 65 | 28.931 | 10.983 | 50.845 | 1.00 | 32.72 | C |
| ATOM | 2374 | O | ILE | B | 65 | 29.264 | 10.555 | 51.952 | 1.00 | 32.24 | O |
| ATOM | 2375 | CB | ILE | B | 65 | 26.665 | 11.997 | 50.392 | 1.00 | 33.23 | C |
| ATOM | 2376 | CG1 | ILE | B | 65 | 25.867 | 13.301 | 50.307 | 1.00 | 32.72 | C |
| ATOM | 2377 | CD1 | ILE | B | 65 | 24.615 | 13.193 | 49.467 | 1.00 | 33.11 | C |
| ATOM | 2378 | CG2 | ILE | B | 65 | 26.048 | 11.033 | 51.425 | 1.00 | 32.17 | C |
| ATOM | 2379 | N | LEU | B | 66 | 29.228 | 10.369 | 49.702 | 1.00 | 32.43 | N |
| ATOM | 2380 | CA | LEU | B | 66 | 29.873 | 9.060 | 49.677 | 1.00 | 32.09 | C |
| ATOM | 2381 | C | LEU | B | 66 | 31.321 | 9.119 | 50.140 | 1.00 | 31.93 | C |
| ATOM | 2382 | O | LEU | B | 66 | 31.779 | 8.215 | 50.840 | 1.00 | 31.40 | O |
| ATOM | 2383 | CB | LEU | B | 66 | 29.775 | 8.431 | 48.290 | 1.00 | 31.89 | C |
| ATOM | 2384 | CG | LEU | B | 66 | 28.393 | 7.923 | 47.888 | 1.00 | 32.00 | C |
| ATOM | 2385 | CD1 | LEU | B | 66 | 28.381 | 7.627 | 46.406 | 1.00 | 32.67 | C |
| ATOM | 2386 | CD2 | LEU | B | 66 | 27.987 | 6.684 | 48.679 | 1.00 | 32.68 | C |
| ATOM | 2387 | N | ASP | B | 67 | 32.026 | 10.184 | 49.750 | 1.00 | 31.87 | N |
| ATOM | 2388 | CA | ASP | B | 67 | 33.398 | 10.432 | 50.207 | 1.00 | 31.89 | C |
| ATOM | 2389 | C | ASP | B | 67 | 33.453 | 10.574 | 51.724 | 1.00 | 31.37 | C |
| ATOM | 2390 | O | ASP | B | 67 | 34.335 | 10.010 | 52.371 | 1.00 | 31.49 | O |
| ATOM | 2391 | CB | ASP | B | 67 | 33.989 | 11.681 | 49.541 | 1.00 | 32.19 | C |
| ATOM | 2392 | CG | ASP | B | 67 | 34.594 | 11.391 | 48.169 | 1.00 | 32.97 | C |
| ATOM | 2393 | OD1 | ASP | B | 67 | 34.807 | 10.207 | 47.822 | 1.00 | 34.04 | O |
| ATOM | 2394 | OD2 | ASP | B | 67 | 34.883 | 12.295 | 47.364 | 1.00 | 33.98 | O |

FIG. 5NN

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2395 | N | GLU | B | 68 | 32.503 | 11.325 | 52.277 | 1.00 | 30.71 | N |
| ATOM | 2396 | CA | GLU | B | 68 | 32.314 | 11.414 | 53.720 | 1.00 | 30.05 | C |
| ATOM | 2397 | C | GLU | B | 68 | 31.983 | 10.046 | 54.321 | 1.00 | 29.64 | C |
| ATOM | 2398 | O | GLU | B | 68 | 32.545 | 9.665 | 55.349 | 1.00 | 29.65 | O |
| ATOM | 2399 | CB | GLU | B | 68 | 31.213 | 12.423 | 54.056 | 1.00 | 30.08 | C |
| ATOM | 2400 | N | ALA | B | 69 | 31.085 | 9.306 | 53.667 | 1.00 | 28.81 | N |
| ATOM | 2401 | CA | ALA | B | 69 | 30.638 | 8.005 | 54.175 | 1.00 | 28.17 | C |
| ATOM | 2402 | C | ALA | B | 69 | 31.765 | 6.973 | 54.233 | 1.00 | 27.40 | C |
| ATOM | 2403 | O | ALA | B | 69 | 31.764 | 6.109 | 55.110 | 1.00 | 27.34 | O |
| ATOM | 2404 | CB | ALA | B | 69 | 29.453 | 7.473 | 53.360 | 1.00 | 27.86 | C |
| ATOM | 2405 | N | TYR | B | 70 | 32.708 | 7.070 | 53.293 | 1.00 | 26.83 | N |
| ATOM | 2406 | CA | TYR | B | 70 | 33.913 | 6.241 | 53.281 | 1.00 | 26.18 | C |
| ATOM | 2407 | C | TYR | B | 70 | 34.724 | 6.441 | 54.563 | 1.00 | 25.63 | C |
| ATOM | 2408 | O | TYR | B | 70 | 34.999 | 5.487 | 55.290 | 1.00 | 25.75 | O |
| ATOM | 2409 | CB | TYR | B | 70 | 34.784 | 6.573 | 52.063 | 1.00 | 26.20 | C |
| ATOM | 2410 | N | VAL | B | 71 | 35.105 | 7.687 | 54.827 | 1.00 | 24.50 | N |
| ATOM | 2411 | CA | VAL | B | 71 | 35.759 | 8.048 | 56.083 | 1.00 | 23.93 | C |
| ATOM | 2412 | C | VAL | B | 71 | 35.008 | 7.436 | 57.277 | 1.00 | 23.40 | C |
| ATOM | 2413 | O | VAL | B | 71 | 35.594 | 6.686 | 58.054 | 1.00 | 23.33 | O |
| ATOM | 2414 | CB | VAL | B | 71 | 35.896 | 9.582 | 56.215 | 1.00 | 23.65 | C |
| ATOM | 2415 | CG1 | VAL | B | 71 | 36.481 | 9.963 | 57.557 | 1.00 | 24.23 | C |
| ATOM | 2416 | CG2 | VAL | B | 71 | 36.758 | 10.135 | 55.086 | 1.00 | 22.88 | C |
| ATOM | 2417 | N | MET | B | 72 | 33.704 | 7.707 | 57.375 | 1.00 | 22.98 | N |
| ATOM | 2418 | CA | MET | B | 72 | 32.867 | 7.205 | 58.472 | 1.00 | 22.35 | C |
| ATOM | 2419 | C | MET | B | 72 | 32.937 | 5.700 | 58.691 | 1.00 | 22.28 | C |
| ATOM | 2420 | O | MET | B | 72 | 32.876 | 5.232 | 59.836 | 1.00 | 21.97 | O |
| ATOM | 2421 | CB | MET | B | 72 | 31.413 | 7.621 | 58.293 | 1.00 | 22.55 | C |
| ATOM | 2422 | CG | MET | B | 72 | 31.153 | 9.106 | 58.455 | 1.00 | 23.54 | C |
| ATOM | 2423 | SD | MET | B | 72 | 29.707 | 9.594 | 57.495 | 1.00 | 25.55 | S |
| ATOM | 2424 | CE | MET | B | 72 | 28.386 | 9.081 | 58.572 | 1.00 | 23.25 | C |
| ATOM | 2425 | N | ALA | B | 73 | 33.075 | 4.958 | 57.588 | 1.00 | 21.57 | N |
| ATOM | 2426 | CA | ALA | B | 73 | 33.123 | 3.499 | 57.592 | 1.00 | 20.92 | C |
| ATOM | 2427 | C | ALA | B | 73 | 34.492 | 2.917 | 57.943 | 1.00 | 20.93 | C |
| ATOM | 2428 | O | ALA | B | 73 | 34.629 | 1.701 | 58.161 | 1.00 | 20.50 | O |
| ATOM | 2429 | CB | ALA | B | 73 | 32.667 | 2.969 | 56.243 | 1.00 | 20.91 | C |
| ATOM | 2430 | N | SER | B | 74 | 35.507 | 3.775 | 57.967 | 1.00 | 21.07 | N |
| ATOM | 2431 | CA | SER | B | 74 | 36.868 | 3.358 | 58.267 | 1.00 | 21.12 | C |
| ATOM | 2432 | C | SER | B | 74 | 37.177 | 3.439 | 59.776 | 1.00 | 21.58 | C |
| ATOM | 2433 | O | SER | B | 74 | 38.204 | 2.937 | 60.237 | 1.00 | 21.30 | O |
| ATOM | 2434 | CB | SER | B | 74 | 37.853 | 4.223 | 57.483 | 1.00 | 21.34 | C |
| ATOM | 2435 | OG | SER | B | 74 | 37.886 | 5.542 | 58.000 | 1.00 | 20.80 | O |
| ATOM | 2436 | N | VAL | B | 75 | 36.285 | 4.073 | 60.534 | 1.00 | 21.73 | N |
| ATOM | 2437 | CA | VAL | B | 75 | 36.480 | 4.261 | 61.969 | 1.00 | 22.25 | C |
| ATOM | 2438 | C | VAL | B | 75 | 36.382 | 2.920 | 62.702 | 1.00 | 22.43 | C |
| ATOM | 2439 | O | VAL | B | 75 | 35.314 | 2.312 | 62.767 | 1.00 | 22.56 | O |
| ATOM | 2440 | CB | VAL | B | 75 | 35.468 | 5.288 | 62.547 | 1.00 | 22.60 | C |
| ATOM | 2441 | CG1 | VAL | B | 75 | 35.373 | 5.161 | 64.045 | 1.00 | 22.97 | C |
| ATOM | 2442 | CG2 | VAL | B | 75 | 35.871 | 6.702 | 62.162 | 1.00 | 21.91 | C |
| ATOM | 2443 | N | ASP | B | 76 | 37.505 | 2.464 | 63.241 | 1.00 | 22.26 | N |
| ATOM | 2444 | CA | ASP | B | 76 | 37.575 | 1.147 | 63.857 | 1.00 | 22.70 | C |
| ATOM | 2445 | C | ASP | B | 76 | 38.123 | 1.219 | 65.286 | 1.00 | 21.92 | C |
| ATOM | 2446 | O | ASP | B | 76 | 39.325 | 1.091 | 65.523 | 1.00 | 21.82 | O |
| ATOM | 2447 | CB | ASP | B | 76 | 38.410 | 0.201 | 62.980 | 1.00 | 23.88 | C |
| ATOM | 2448 | CG | ASP | B | 76 | 38.331 | -1.239 | 63.432 | 1.00 | 25.38 | C |
| ATOM | 2449 | OD1 | ASP | B | 76 | 37.334 | -1.612 | 64.086 | 1.00 | 28.10 | O |
| ATOM | 2450 | OD2 | ASP | B | 76 | 39.222 | -2.076 | 63.184 | 1.00 | 28.14 | O |
| ATOM | 2451 | N | ASN | B | 77 | 37.211 | 1.449 | 66.222 | 1.00 | 20.75 | N |
| ATOM | 2452 | CA | ASN | B | 77 | 37.519 | 1.570 | 67.632 | 1.00 | 19.45 | C |
| ATOM | 2453 | C | ASN | B | 77 | 36.298 | 1.114 | 68.421 | 1.00 | 18.63 | C |
| ATOM | 2454 | O | ASN | B | 77 | 35.176 | 1.410 | 68.020 | 1.00 | 18.76 | O |

FIG. 500

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2455 | CB | ASN | B | 77 | 37.852 | 3.021 | 67.978 | 1.00 | 19.30 | C |
| ATOM | 2456 | CG | ASN | B | 77 | 38.111 | 3.217 | 69.455 | 1.00 | 19.07 | C |
| ATOM | 2457 | OD1 | ASN | B | 77 | 37.210 | 3.558 | 70.219 | 1.00 | 18.90 | O |
| ATOM | 2458 | ND2 | ASN | B | 77 | 39.338 | 2.961 | 69.872 | 1.00 | 19.78 | N |
| ATOM | 2459 | N | PRO | B | 78 | 36.503 | 0.403 | 69.531 | 1.00 | 18.22 | N |
| ATOM | 2460 | CA | PRO | B | 78 | 35.381 | -0.112 | 70.338 | 1.00 | 17.65 | C |
| ATOM | 2461 | C | PRO | B | 78 | 34.465 | 0.970 | 70.925 | 1.00 | 17.30 | C |
| ATOM | 2462 | O | PRO | B | 78 | 33.376 | 0.636 | 71.380 | 1.00 | 17.27 | O |
| ATOM | 2463 | CB | PRO | B | 78 | 36.077 | -0.875 | 71.476 | 1.00 | 17.40 | C |
| ATOM | 2464 | CG | PRO | B | 78 | 37.469 | -1.111 | 71.003 | 1.00 | 17.81 | C |
| ATOM | 2465 | CD | PRO | B | 78 | 37.814 | 0.015 | 70.091 | 1.00 | 17.79 | C |
| ATOM | 2466 | N | HIS | B | 79 | 34.886 | 2.231 | 70.903 | 1.00 | 16.76 | N |
| ATOM | 2467 | CA | HIS | B | 79 | 34.107 | 3.298 | 71.511 | 1.00 | 16.62 | C |
| ATOM | 2468 | C | HIS | B | 79 | 33.640 | 4.376 | 70.540 | 1.00 | 17.28 | C |
| ATOM | 2469 | O | HIS | B | 79 | 33.203 | 5.455 | 70.957 | 1.00 | 16.78 | O |
| ATOM | 2470 | CB | HIS | B | 79 | 34.863 | 3.884 | 72.699 | 1.00 | 16.25 | C |
| ATOM | 2471 | CG | HIS | B | 79 | 35.187 | 2.864 | 73.739 | 1.00 | 15.59 | C |
| ATOM | 2472 | ND1 | HIS | B | 79 | 34.214 | 2.225 | 74.477 | 1.00 | 15.58 | N |
| ATOM | 2473 | CE1 | HIS | B | 79 | 34.783 | 1.360 | 75.295 | 1.00 | 15.24 | C |
| ATOM | 2474 | NE2 | HIS | B | 79 | 36.090 | 1.407 | 75.106 | 1.00 | 15.70 | N |
| ATOM | 2475 | CD2 | HIS | B | 79 | 36.367 | 2.330 | 74.128 | 1.00 | 15.23 | C |
| ATOM | 2476 | N | VAL | B | 80 | 33.731 | 4.071 | 69.247 | 1.00 | 18.09 | N |
| ATOM | 2477 | CA | VAL | B | 80 | 33.107 | 4.882 | 68.203 | 1.00 | 19.06 | C |
| ATOM | 2478 | C | VAL | B | 80 | 32.332 | 3.958 | 67.255 | 1.00 | 19.99 | C |
| ATOM | 2479 | O | VAL | B | 80 | 32.827 | 2.885 | 66.875 | 1.00 | 20.37 | O |
| ATOM | 2480 | CB | VAL | B | 80 | 34.141 | 5.727 | 67.408 | 1.00 | 19.07 | C |
| ATOM | 2481 | CG1 | VAL | B | 80 | 33.440 | 6.716 | 66.492 | 1.00 | 18.71 | C |
| ATOM | 2482 | CG2 | VAL | B | 80 | 35.099 | 6.480 | 68.349 | 1.00 | 18.69 | C |
| ATOM | 2483 | N | CYS | B | 81 | 31.115 | 4.369 | 66.902 | 1.00 | 20.57 | N |
| ATOM | 2484 | CA | CYS | B | 81 | 30.274 | 3.661 | 65.932 | 1.00 | 21.04 | C |
| ATOM | 2485 | C | CYS | B | 81 | 30.789 | 3.803 | 64.492 | 1.00 | 21.16 | C |
| ATOM | 2486 | O | CYS | B | 81 | 30.920 | 4.919 | 63.973 | 1.00 | 20.67 | O |
| ATOM | 2487 | CB | CYS | B | 81 | 28.850 | 4.208 | 65.987 | 1.00 | 20.66 | C |
| ATOM | 2488 | SG | CYS | B | 81 | 27.968 | 3.883 | 67.528 | 1.00 | 24.94 | S |
| ATOM | 2489 | N | ARG | B | 82 | 31.062 | 2.677 | 63.840 | 1.00 | 21.12 | N |
| ATOM | 2490 | CA | ARG | B | 82 | 31.383 | 2.712 | 62.415 | 1.00 | 21.57 | C |
| ATOM | 2491 | C | ARG | B | 82 | 30.149 | 2.585 | 61.536 | 1.00 | 21.20 | C |
| ATOM | 2492 | O | ARG | B | 82 | 29.220 | 1.834 | 61.857 | 1.00 | 20.65 | O |
| ATOM | 2493 | CB | ARG | B | 82 | 32.442 | 1.672 | 62.015 | 1.00 | 21.61 | C |
| ATOM | 2494 | CG | ARG | B | 82 | 32.103 | 0.224 | 62.254 | 1.00 | 24.13 | C |
| ATOM | 2495 | CD | ARG | B | 82 | 33.068 | -0.757 | 61.551 | 1.00 | 25.41 | C |
| ATOM | 2496 | NE | ARG | B | 82 | 33.310 | -0.339 | 60.175 | 1.00 | 26.67 | N |
| ATOM | 2497 | CZ | ARG | B | 82 | 33.087 | -1.094 | 59.099 | 1.00 | 27.89 | C |
| ATOM | 2498 | NH1 | ARG | B | 82 | 33.321 | -0.606 | 57.887 | 1.00 | 27.21 | N |
| ATOM | 2499 | NH2 | ARG | B | 82 | 32.635 | -2.336 | 59.226 | 1.00 | 28.49 | N |
| ATOM | 2500 | N | LEU | B | 83 | 30.158 | 3.326 | 60.430 | 1.00 | 20.59 | N |
| ATOM | 2501 | CA | LEU | B | 83 | 29.180 | 3.146 | 59.371 | 1.00 | 21.03 | C |
| ATOM | 2502 | C | LEU | B | 83 | 29.392 | 1.808 | 58.664 | 1.00 | 21.12 | C |
| ATOM | 2503 | O | LEU | B | 83 | 30.474 | 1.547 | 58.128 | 1.00 | 21.23 | O |
| ATOM | 2504 | CB | LEU | B | 83 | 29.262 | 4.291 | 58.355 | 1.00 | 20.75 | C |
| ATOM | 2505 | CG | LEU | B | 83 | 28.126 | 4.305 | 57.323 | 1.00 | 20.46 | C |
| ATOM | 2506 | CD1 | LEU | B | 83 | 26.777 | 4.404 | 58.020 | 1.00 | 18.57 | C |
| ATOM | 2507 | CD2 | LEU | B | 83 | 28.306 | 5.437 | 56.324 | 1.00 | 20.59 | C |
| ATOM | 2508 | N | LEU | B | 84 | 28.361 | 0.966 | 58.672 | 1.00 | 21.46 | N |
| ATOM | 2509 | CA | LEU | B | 84 | 28.424 | -0.332 | 57.993 | 1.00 | 21.83 | C |
| ATOM | 2510 | C | LEU | B | 84 | 28.043 | -0.215 | 56.524 | 1.00 | 22.01 | C |
| ATOM | 2511 | O | LEU | B | 84 | 28.692 | -0.808 | 55.662 | 1.00 | 22.89 | O |
| ATOM | 2512 | CB | LEU | B | 84 | 27.535 | -1.367 | 58.688 | 1.00 | 21.87 | C |
| ATOM | 2513 | CG | LEU | B | 84 | 27.909 | -1.870 | 60.091 | 1.00 | 22.94 | C |
| ATOM | 2514 | CD1 | LEU | B | 84 | 27.063 | -3.086 | 60.458 | 1.00 | 22.71 | C |

FIG. 5PP

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2515 | CD2 | LEU | B | 84 | 29.400 | -2.209 | 60.202 | 1.00 | 23.06 | C |
| ATOM | 2516 | N | GLY | B | 85 | 26.993 | 0.556 | 56.246 | 1.00 | 21.90 | N |
| ATOM | 2517 | CA | GLY | B | 85 | 26.523 | 0.764 | 54.887 | 1.00 | 21.72 | C |
| ATOM | 2518 | C | GLY | B | 85 | 25.743 | 2.051 | 54.657 | 1.00 | 21.48 | C |
| ATOM | 2519 | O | GLY | B | 85 | 25.283 | 2.708 | 55.592 | 1.00 | 20.43 | O |
| ATOM | 2520 | N | ILE | B | 86 | 25.609 | 2.414 | 53.388 | 1.00 | 22.03 | N |
| ATOM | 2521 | CA | ILE | B | 86 | 24.823 | 3.576 | 52.993 | 1.00 | 23.02 | C |
| ATOM | 2522 | C | ILE | B | 86 | 23.897 | 3.230 | 51.834 | 1.00 | 23.29 | C |
| ATOM | 2523 | O | ILE | B | 86 | 24.248 | 2.443 | 50.962 | 1.00 | 23.90 | O |
| ATOM | 2524 | CB | ILE | B | 86 | 25.748 | 4.787 | 52.655 | 1.00 | 22.54 | C |
| ATOM | 2525 | CG1 | ILE | B | 86 | 24.923 | 6.037 | 52.322 | 1.00 | 22.40 | C |
| ATOM | 2526 | CD1 | ILE | B | 86 | 25.665 | 7.360 | 52.519 | 1.00 | 20.16 | C |
| ATOM | 2527 | CG2 | ILE | B | 86 | 26.748 | 4.434 | 51.547 | 1.00 | 23.46 | C |
| ATOM | 2528 | N | CYS | B | 87 | 22.711 | 3.828 | 51.837 | 1.00 | 24.14 | N |
| ATOM | 2529 | CA | CYS | B | 87 | 21.762 | 3.680 | 50.744 | 1.00 | 24.38 | C |
| ATOM | 2530 | C | CYS | B | 87 | 21.235 | 5.041 | 50.329 | 1.00 | 24.49 | C |
| ATOM | 2531 | O | CYS | B | 87 | 20.686 | 5.771 | 51.159 | 1.00 | 24.32 | O |
| ATOM | 2532 | CB | CYS | B | 87 | 20.600 | 2.779 | 51.154 | 1.00 | 23.75 | C |
| ATOM | 2533 | SG | CYS | B | 87 | 19.374 | 2.580 | 49.848 | 1.00 | 25.50 | S |
| ATOM | 2534 | N | LEU | B | 88 | 21.401 | 5.367 | 49.047 | 1.00 | 24.76 | N |
| ATOM | 2535 | CA | LEU | B | 88 | 20.933 | 6.643 | 48.496 | 1.00 | 25.70 | C |
| ATOM | 2536 | C | LEU | B | 88 | 19.710 | 6.471 | 47.606 | 1.00 | 26.24 | C |
| ATOM | 2537 | O | LEU | B | 88 | 19.830 | 6.040 | 46.459 | 1.00 | 27.00 | O |
| ATOM | 2538 | CB | LEU | B | 88 | 22.035 | 7.357 | 47.699 | 1.00 | 25.41 | C |
| ATOM | 2539 | CG | LEU | B | 88 | 23.445 | 7.532 | 48.285 | 1.00 | 26.65 | C |
| ATOM | 2540 | CD1 | LEU | B | 88 | 24.448 | 7.779 | 47.158 | 1.00 | 26.03 | C |
| ATOM | 2541 | CD2 | LEU | B | 88 | 23.505 | 8.658 | 49.318 | 1.00 | 25.11 | C |
| ATOM | 2542 | N | THR | B | 89 | 18.534 | 6.789 | 48.143 | 1.00 | 26.96 | N |
| ATOM | 2543 | CA | THR | B | 89 | 17.317 | 6.883 | 47.339 | 1.00 | 27.40 | C |
| ATOM | 2544 | C | THR | B | 89 | 16.668 | 8.240 | 47.589 | 1.00 | 27.88 | C |
| ATOM | 2545 | O | THR | B | 89 | 17.355 | 9.258 | 47.554 | 1.00 | 29.14 | O |
| ATOM | 2546 | CB | THR | B | 89 | 16.347 | 5.709 | 47.604 | 1.00 | 27.45 | C |
| ATOM | 2547 | OG1 | THR | B | 89 | 16.151 | 5.544 | 49.013 | 1.00 | 27.64 | O |
| ATOM | 2548 | CG2 | THR | B | 89 | 16.967 | 4.383 | 47.171 | 1.00 | 26.98 | C |
| ATOM | 2549 | N | SER | B | 90 | 15.363 | 8.274 | 47.835 | 1.00 | 28.04 | N |
| ATOM | 2550 | CA | SER | B | 90 | 14.683 | 9.538 | 48.128 | 1.00 | 27.95 | C |
| ATOM | 2551 | C | SER | B | 90 | 15.281 | 10.176 | 49.384 | 1.00 | 27.91 | C |
| ATOM | 2552 | O | SER | B | 90 | 15.338 | 11.402 | 49.513 | 1.00 | 27.35 | O |
| ATOM | 2553 | CB | SER | B | 90 | 13.178 | 9.322 | 48.301 | 1.00 | 27.76 | C |
| ATOM | 2554 | N | THR | B | 91 | 15.726 | 9.324 | 50.304 | 1.00 | 27.53 | N |
| ATOM | 2555 | CA | THR | B | 91 | 16.449 | 9.768 | 51.487 | 1.00 | 27.38 | C |
| ATOM | 2556 | C | THR | B | 91 | 17.796 | 9.074 | 51.494 | 1.00 | 26.76 | C |
| ATOM | 2557 | O | THR | B | 91 | 17.957 | 8.045 | 50.843 | 1.00 | 27.69 | O |
| ATOM | 2558 | CB | THR | B | 91 | 15.676 | 9.378 | 52.758 | 1.00 | 27.65 | C |
| ATOM | 2559 | OG1 | THR | B | 91 | 15.419 | 7.964 | 52.738 | 1.00 | 28.16 | O |
| ATOM | 2560 | CG2 | THR | B | 91 | 14.273 | 10.009 | 52.781 | 1.00 | 27.34 | C |
| ATOM | 2561 | N | VAL | B | 92 | 18.765 | 9.628 | 52.215 | 1.00 | 26.07 | N |
| ATOM | 2562 | CA | VAL | B | 92 | 19.963 | 8.859 | 52.555 | 1.00 | 25.56 | C |
| ATOM | 2563 | C | VAL | B | 92 | 19.701 | 8.055 | 53.840 | 1.00 | 25.11 | C |
| ATOM | 2564 | O | VAL | B | 92 | 19.095 | 8.554 | 54.789 | 1.00 | 25.18 | O |
| ATOM | 2565 | CB | VAL | B | 92 | 21.276 | 9.726 | 52.590 | 1.00 | 25.80 | C |
| ATOM | 2566 | CG1 | VAL | B | 92 | 20.970 | 11.215 | 52.652 | 1.00 | 26.18 | C |
| ATOM | 2567 | CG2 | VAL | B | 92 | 22.228 | 9.299 | 53.710 | 1.00 | 25.19 | C |
| ATOM | 2568 | N | GLN | B | 93 | 20.127 | 6.797 | 53.837 | 1.00 | 24.35 | N |
| ATOM | 2569 | CA | GLN | B | 93 | 19.879 | 5.882 | 54.946 | 1.00 | 23.94 | C |
| ATOM | 2570 | C | GLN | B | 93 | 21.175 | 5.218 | 55.374 | 1.00 | 23.50 | C |
| ATOM | 2571 | O | GLN | B | 93 | 21.879 | 4.617 | 54.557 | 1.00 | 23.29 | O |
| ATOM | 2572 | CB | GLN | B | 93 | 18.855 | 4.812 | 54.553 | 1.00 | 23.94 | C |
| ATOM | 2573 | CG | GLN | B | 93 | 17.436 | 5.322 | 54.364 | 1.00 | 24.30 | C |
| ATOM | 2574 | CD | GLN | B | 93 | 16.438 | 4.194 | 54.220 | 1.00 | 25.21 | C |

FIG. 5QQ

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2575 | OE1 | GLN | B | 93 | 15.989 | 3.627 | 55.217 | 1.00 | 25.55 | O |
| ATOM | 2576 | NE2 | GLN | B | 93 | 16.101 | 3.852 | 52.985 | 1.00 | 25.37 | N |
| ATOM | 2577 | N | LEU | B | 94 | 21.487 | 5.324 | 56.660 | 1.00 | 23.14 | N |
| ATOM | 2578 | CA | LEU | B | 94 | 22.754 | 4.817 | 57.171 | 1.00 | 22.90 | C |
| ATOM | 2579 | C | LEU | B | 94 | 22.538 | 3.572 | 58.013 | 1.00 | 22.73 | C |
| ATOM | 2580 | O | LEU | B | 94 | 21.736 | 3.574 | 58.944 | 1.00 | 22.24 | O |
| ATOM | 2581 | CB | LEU | B | 94 | 23.487 | 5.893 | 57.973 | 1.00 | 22.86 | C |
| ATOM | 2582 | CG | LEU | B | 94 | 23.767 | 7.250 | 57.317 | 1.00 | 23.23 | C |
| ATOM | 2583 | CD1 | LEU | B | 94 | 24.284 | 8.221 | 58.362 | 1.00 | 21.95 | C |
| ATOM | 2584 | CD2 | LEU | B | 94 | 24.766 | 7.146 | 56.151 | 1.00 | 23.29 | C |
| ATOM | 2585 | N | ILE | B | 95 | 23.264 | 2.512 | 57.670 | 1.00 | 22.93 | N |
| ATOM | 2586 | CA | ILE | B | 95 | 23.153 | 1.233 | 58.358 | 1.00 | 23.65 | C |
| ATOM | 2587 | C | ILE | B | 95 | 24.368 | 1.058 | 59.268 | 1.00 | 24.36 | C |
| ATOM | 2588 | O | ILE | B | 95 | 25.505 | 1.207 | 58.824 | 1.00 | 24.72 | O |
| ATOM | 2589 | CB | ILE | B | 95 | 23.025 | 0.059 | 57.328 | 1.00 | 23.42 | C |
| ATOM | 2590 | CG1 | ILE | B | 95 | 21.623 | 0.024 | 56.701 | 1.00 | 22.82 | C |
| ATOM | 2591 | CD1 | ILE | B | 95 | 21.383 | 1.054 | 55.590 | 1.00 | 21.22 | C |
| ATOM | 2592 | CG2 | ILE | B | 95 | 23.322 | -1.289 | 57.989 | 1.00 | 22.89 | C |
| ATOM | 2593 | N | THR | B | 96 | 24.112 | 0.775 | 60.543 | 1.00 | 25.04 | N |
| ATOM | 2594 | CA | THR | B | 96 | 25.165 | 0.560 | 61.538 | 1.00 | 26.08 | C |
| ATOM | 2595 | C | THR | B | 96 | 24.816 | -0.623 | 62.431 | 1.00 | 26.75 | C |
| ATOM | 2596 | O | THR | B | 96 | 23.778 | -1.276 | 62.252 | 1.00 | 26.73 | O |
| ATOM | 2597 | CB | THR | B | 96 | 25.361 | 1.811 | 62.435 | 1.00 | 26.32 | C |
| ATOM | 2598 | OG1 | THR | B | 96 | 24.198 | 1.995 | 63.258 | 1.00 | 26.97 | O |
| ATOM | 2599 | CG2 | THR | B | 96 | 25.446 | 3.098 | 61.611 | 1.00 | 25.72 | C |
| ATOM | 2600 | N | GLN | B | 97 | 25.682 | -0.882 | 63.407 | 1.00 | 27.33 | N |
| ATOM | 2601 | CA | GLN | B | 97 | 25.415 | -1.893 | 64.416 | 1.00 | 27.72 | C |
| ATOM | 2602 | C | GLN | B | 97 | 24.342 | -1.396 | 65.382 | 1.00 | 27.90 | C |
| ATOM | 2603 | O | GLN | B | 97 | 24.411 | -0.272 | 65.888 | 1.00 | 27.68 | O |
| ATOM | 2604 | CB | GLN | B | 97 | 26.692 | -2.249 | 65.175 | 1.00 | 27.95 | C |
| ATOM | 2605 | CG | GLN | B | 97 | 26.575 | -3.505 | 66.030 | 1.00 | 28.85 | C |
| ATOM | 2606 | CD | GLN | B | 97 | 27.791 | -3.733 | 66.898 | 1.00 | 30.48 | C |
| ATOM | 2607 | OE1 | GLN | B | 97 | 28.927 | -3.699 | 66.415 | 1.00 | 30.45 | O |
| ATOM | 2608 | NE2 | GLN | B | 97 | 27.562 | -3.976 | 68.182 | 1.00 | 31.15 | N |
| ATOM | 2609 | N | LEU | B | 98 | 23.353 | -2.249 | 65.628 | 1.00 | 27.99 | N |
| ATOM | 2610 | CA | LEU | B | 98 | 22.275 | -1.946 | 66.560 | 1.00 | 28.25 | C |
| ATOM | 2611 | C | LEU | B | 98 | 22.820 | -1.773 | 67.973 | 1.00 | 28.10 | C |
| ATOM | 2612 | O | LEU | B | 98 | 23.499 | -2.651 | 68.497 | 1.00 | 28.46 | O |
| ATOM | 2613 | CB | LEU | B | 98 | 21.226 | -3.062 | 66.525 | 1.00 | 28.18 | C |
| ATOM | 2614 | CG | LEU | B | 98 | 20.001 | -2.977 | 67.431 | 1.00 | 28.87 | C |
| ATOM | 2615 | CD1 | LEU | B | 98 | 18.983 | -2.028 | 66.857 | 1.00 | 29.73 | C |
| ATOM | 2616 | CD2 | LEU | B | 98 | 19.403 | -4.355 | 67.593 | 1.00 | 29.80 | C |
| ATOM | 2617 | N | MET | B | 99 | 22.540 | -0.626 | 68.578 | 1.00 | 27.86 | N |
| ATOM | 2618 | CA | MET | B | 99 | 22.921 | -0.406 | 69.963 | 1.00 | 27.53 | C |
| ATOM | 2619 | C | MET | B | 99 | 21.686 | -0.425 | 70.861 | 1.00 | 27.17 | C |
| ATOM | 2620 | O | MET | B | 99 | 20.962 | 0.565 | 70.976 | 1.00 | 27.76 | O |
| ATOM | 2621 | CB | MET | B | 99 | 23.763 | 0.852 | 70.120 | 1.00 | 27.77 | C |
| ATOM | 2622 | CG | MET | B | 99 | 25.065 | 0.538 | 70.820 | 1.00 | 28.91 | C |
| ATOM | 2623 | SD | MET | B | 99 | 26.547 | 0.790 | 69.889 | 1.00 | 29.11 | S |
| ATOM | 2624 | CE | MET | B | 99 | 26.574 | -0.601 | 68.791 | 1.00 | 29.87 | C |
| ATOM | 2625 | N | PRO | B | 100 | 21.456 | -1.589 | 71.468 | 1.00 | 26.21 | N |
| ATOM | 2626 | CA | PRO | B | 100 | 20.168 | -1.968 | 72.065 | 1.00 | 25.16 | C |
| ATOM | 2627 | C | PRO | B | 100 | 19.660 | -1.162 | 73.262 | 1.00 | 24.07 | C |
| ATOM | 2628 | O | PRO | B | 100 | 18.461 | -1.184 | 73.521 | 1.00 | 23.91 | O |
| ATOM | 2629 | CB | PRO | B | 100 | 20.415 | -3.422 | 72.491 | 1.00 | 25.31 | C |
| ATOM | 2630 | CG | PRO | B | 100 | 21.538 | -3.873 | 71.610 | 1.00 | 25.47 | C |
| ATOM | 2631 | CD | PRO | B | 100 | 22.442 | -2.677 | 71.584 | 1.00 | 26.61 | C |
| ATOM | 2632 | N | PHE | B | 101 | 20.532 | -0.483 | 73.994 | 1.00 | 23.55 | N |
| ATOM | 2633 | CA | PHE | B | 101 | 20.065 | 0.315 | 75.129 | 1.00 | 21.97 | C |
| ATOM | 2634 | C | PHE | B | 101 | 19.858 | 1.783 | 74.748 | 1.00 | 21.55 | C |

FIG. 5RR

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2635 | O | PHE | B | 101 | 19.432 | 2.605 | 75.566 | 1.00 | 21.46 | O |
| ATOM | 2636 | CB | PHE | B | 101 | 20.990 | 0.149 | 76.328 | 1.00 | 21.63 | C |
| ATOM | 2637 | CG | PHE | B | 101 | 20.986 | -1.237 | 76.910 | 1.00 | 20.98 | C |
| ATOM | 2638 | CD1 | PHE | B | 101 | 20.123 | -1.573 | 77.951 | 1.00 | 20.86 | C |
| ATOM | 2639 | CE1 | PHE | B | 101 | 20.129 | -2.862 | 78.495 | 1.00 | 20.19 | C |
| ATOM | 2640 | CZ | PHE | B | 101 | 21.006 | -3.819 | 78.002 | 1.00 | 19.17 | C |
| ATOM | 2641 | CE2 | PHE | B | 101 | 21.865 | -3.492 | 76.969 | 1.00 | 20.10 | C |
| ATOM | 2642 | CD2 | PHE | B | 101 | 21.852 | -2.205 | 76.429 | 1.00 | 20.98 | C |
| ATOM | 2643 | N | GLY | B | 102 | 20.145 | 2.097 | 73.490 | 1.00 | 20.66 | N |
| ATOM | 2644 | CA | GLY | B | 102 | 19.847 | 3.406 | 72.949 | 1.00 | 20.06 | C |
| ATOM | 2645 | C | GLY | B | 102 | 20.822 | 4.498 | 73.346 | 1.00 | 20.02 | C |
| ATOM | 2646 | O | GLY | B | 102 | 22.015 | 4.270 | 73.558 | 1.00 | 19.74 | O |
| ATOM | 2647 | N | CYS | B | 103 | 20.279 | 5.698 | 73.454 | 1.00 | 19.12 | N |
| ATOM | 2648 | CA | CYS | B | 103 | 21.035 | 6.907 | 73.683 | 1.00 | 19.11 | C |
| ATOM | 2649 | C | CYS | B | 103 | 21.391 | 7.115 | 75.166 | 1.00 | 18.29 | C |
| ATOM | 2650 | O | CYS | B | 103 | 20.535 | 6.981 | 76.051 | 1.00 | 17.97 | O |
| ATOM | 2651 | CB | CYS | B | 103 | 20.193 | 8.056 | 73.140 | 1.00 | 20.09 | C |
| ATOM | 2652 | SG | CYS | B | 103 | 20.807 | 9.700 | 73.416 | 1.00 | 23.15 | S |
| ATOM | 2653 | N | LEU | B | 104 | 22.660 | 7.440 | 75.427 | 1.00 | 17.12 | N |
| ATOM | 2654 | CA | LEU | B | 104 | 23.153 | 7.655 | 76.790 | 1.00 | 15.63 | C |
| ATOM | 2655 | C | LEU | B | 104 | 22.440 | 8.788 | 77.535 | 1.00 | 15.39 | C |
| ATOM | 2656 | O | LEU | B | 104 | 22.253 | 8.709 | 78.755 | 1.00 | 14.67 | O |
| ATOM | 2657 | CB | LEU | B | 104 | 24.661 | 7.904 | 76.790 | 1.00 | 15.18 | C |
| ATOM | 2658 | CG | LEU | B | 104 | 25.365 | 7.970 | 78.156 | 1.00 | 15.34 | C |
| ATOM | 2659 | CD1 | LEU | B | 104 | 25.218 | 6.674 | 78.974 | 1.00 | 14.66 | C |
| ATOM | 2660 | CD2 | LEU | B | 104 | 26.846 | 8.340 | 77.987 | 1.00 | 16.28 | C |
| ATOM | 2661 | N | LEU | B | 105 | 22.065 | 9.839 | 76.803 | 1.00 | 14.31 | N |
| ATOM | 2662 | CA | LEU | B | 105 | 21.304 | 10.936 | 77.381 | 1.00 | 14.50 | C |
| ATOM | 2663 | C | LEU | B | 105 | 20.001 | 10.439 | 78.012 | 1.00 | 13.83 | C |
| ATOM | 2664 | O | LEU | B | 105 | 19.724 | 10.752 | 79.164 | 1.00 | 13.04 | O |
| ATOM | 2665 | CB | LEU | B | 105 | 21.024 | 12.043 | 76.343 | 1.00 | 14.26 | C |
| ATOM | 2666 | CG | LEU | B | 105 | 20.303 | 13.275 | 76.910 | 1.00 | 14.49 | C |
| ATOM | 2667 | CD1 | LEU | B | 105 | 21.073 | 13.881 | 78.067 | 1.00 | 13.80 | C |
| ATOM | 2668 | CD2 | LEU | B | 105 | 19.998 | 14.322 | 75.845 | 1.00 | 14.77 | C |
| ATOM | 2669 | N | ASP | B | 106 | 19.222 | 9.673 | 77.242 | 1.00 | 14.14 | N |
| ATOM | 2670 | CA | ASP | B | 106 | 17.959 | 9.102 | 77.698 | 1.00 | 15.05 | C |
| ATOM | 2671 | C | ASP | B | 106 | 18.206 | 8.073 | 78.791 | 1.00 | 15.23 | C |
| ATOM | 2672 | O | ASP | B | 106 | 17.441 | 7.974 | 79.751 | 1.00 | 15.20 | O |
| ATOM | 2673 | CB | ASP | B | 106 | 17.196 | 8.455 | 76.533 | 1.00 | 15.46 | C |
| ATOM | 2674 | CG | ASP | B | 106 | 16.851 | 9.448 | 75.438 | 1.00 | 17.25 | C |
| ATOM | 2675 | OD1 | ASP | B | 106 | 16.785 | 9.032 | 74.259 | 1.00 | 19.23 | O |
| ATOM | 2676 | OD2 | ASP | B | 106 | 16.644 | 10.667 | 75.655 | 1.00 | 17.57 | O |
| ATOM | 2677 | N | TYR | B | 107 | 19.295 | 7.328 | 78.649 | 1.00 | 15.49 | N |
| ATOM | 2678 | CA | TYR | B | 107 | 19.653 | 6.317 | 79.624 | 1.00 | 16.54 | C |
| ATOM | 2679 | C | TYR | B | 107 | 19.793 | 6.881 | 81.044 | 1.00 | 16.61 | C |
| ATOM | 2680 | O | TYR | B | 107 | 19.169 | 6.364 | 81.980 | 1.00 | 15.97 | O |
| ATOM | 2681 | CB | TYR | B | 107 | 20.928 | 5.588 | 79.202 | 1.00 | 16.82 | C |
| ATOM | 2682 | CG | TYR | B | 107 | 21.189 | 4.361 | 80.028 | 1.00 | 17.98 | C |
| ATOM | 2683 | CD1 | TYR | B | 107 | 20.532 | 3.163 | 79.757 | 1.00 | 18.47 | C |
| ATOM | 2684 | CE1 | TYR | B | 107 | 20.772 | 2.030 | 80.522 | 1.00 | 19.67 | C |
| ATOM | 2685 | CZ | TYR | B | 107 | 21.668 | 2.095 | 81.570 | 1.00 | 20.24 | C |
| ATOM | 2686 | OH | TYR | B | 107 | 21.911 | 0.977 | 82.339 | 1.00 | 22.83 | O |
| ATOM | 2687 | CE2 | TYR | B | 107 | 22.327 | 3.275 | 81.863 | 1.00 | 19.35 | C |
| ATOM | 2688 | CD2 | TYR | B | 107 | 22.084 | 4.398 | 81.093 | 1.00 | 19.26 | C |
| ATOM | 2689 | N | VAL | B | 108 | 20.590 | 7.945 | 81.190 | 1.00 | 16.66 | N |
| ATOM | 2690 | CA | VAL | B | 108 | 20.836 | 8.556 | 82.497 | 1.00 | 17.11 | C |
| ATOM | 2691 | C | VAL | B | 108 | 19.616 | 9.300 | 83.040 | 1.00 | 18.07 | C |
| ATOM | 2692 | O | VAL | B | 108 | 19.456 | 9.422 | 84.259 | 1.00 | 18.49 | O |
| ATOM | 2693 | CB | VAL | B | 108 | 22.115 | 9.446 | 82.547 | 1.00 | 16.82 | C |
| ATOM | 2694 | CG1 | VAL | B | 108 | 23.351 | 8.640 | 82.139 | 1.00 | 16.10 | C |

FIG. 5SS

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2695 | CG2 | VAL | B | 108 | 21.971 | 10.688 | 81.665 | 1.00 | 16.53 | C |
| ATOM | 2696 | N | ARG | B | 109 | 18.755 | 9.786 | 82.147 | 1.00 | 18.27 | N |
| ATOM | 2697 | CA | ARG | B | 109 | 17.487 | 10.370 | 82.580 | 1.00 | 18.81 | C |
| ATOM | 2698 | C | ARG | B | 109 | 16.569 | 9.280 | 83.111 | 1.00 | 19.62 | C |
| ATOM | 2699 | O | ARG | B | 109 | 15.923 | 9.466 | 84.133 | 1.00 | 19.14 | O |
| ATOM | 2700 | CB | ARG | B | 109 | 16.798 | 11.135 | 81.446 | 1.00 | 18.22 | C |
| ATOM | 2701 | CG | ARG | B | 109 | 17.355 | 12.513 | 81.226 | 1.00 | 17.93 | C |
| ATOM | 2702 | CD | ARG | B | 109 | 16.975 | 13.100 | 79.893 | 1.00 | 17.88 | C |
| ATOM | 2703 | NE | ARG | B | 109 | 17.628 | 14.380 | 79.669 | 1.00 | 17.68 | N |
| ATOM | 2704 | CZ | ARG | B | 109 | 17.462 | 15.125 | 78.584 | 1.00 | 18.11 | C |
| ATOM | 2705 | NH1 | ARG | B | 109 | 16.652 | 14.718 | 77.607 | 1.00 | 16.86 | N |
| ATOM | 2706 | NH2 | ARG | B | 109 | 18.108 | 16.279 | 78.475 | 1.00 | 17.17 | N |
| ATOM | 2707 | N | GLU | B | 110 | 16.541 | 8.140 | 82.417 | 1.00 | 21.12 | N |
| ATOM | 2708 | CA | GLU | B | 110 | 15.657 | 7.028 | 82.760 | 1.00 | 22.63 | C |
| ATOM | 2709 | C | GLU | B | 110 | 16.123 | 6.232 | 83.980 | 1.00 | 22.58 | C |
| ATOM | 2710 | O | GLU | B | 110 | 15.310 | 5.692 | 84.722 | 1.00 | 22.68 | O |
| ATOM | 2711 | CB | GLU | B | 110 | 15.497 | 6.091 | 81.560 | 1.00 | 23.54 | C |
| ATOM | 2712 | CG | GLU | B | 110 | 14.269 | 5.197 | 81.625 | 1.00 | 26.48 | C |
| ATOM | 2713 | CD | GLU | B | 110 | 14.147 | 4.265 | 80.437 | 1.00 | 29.89 | C |
| ATOM | 2714 | OE1 | GLU | B | 110 | 13.825 | 3.072 | 80.655 | 1.00 | 32.31 | O |
| ATOM | 2715 | OE2 | GLU | B | 110 | 14.362 | 4.719 | 79.286 | 1.00 | 31.50 | O |
| ATOM | 2716 | N | HIS | B | 111 | 17.432 | 6.163 | 84.187 | 1.00 | 23.09 | N |
| ATOM | 2717 | CA | HIS | B | 111 | 17.984 | 5.295 | 85.227 | 1.00 | 22.79 | C |
| ATOM | 2718 | C | HIS | B | 111 | 18.700 | 6.039 | 86.349 | 1.00 | 23.14 | C |
| ATOM | 2719 | O | HIS | B | 111 | 19.431 | 5.434 | 87.139 | 1.00 | 23.70 | O |
| ATOM | 2720 | CB | HIS | B | 111 | 18.868 | 4.227 | 84.596 | 1.00 | 22.31 | C |
| ATOM | 2721 | CG | HIS | B | 111 | 18.102 | 3.224 | 83.792 | 1.00 | 22.56 | C |
| ATOM | 2722 | ND1 | HIS | B | 111 | 18.223 | 3.116 | 82.424 | 1.00 | 22.37 | N |
| ATOM | 2723 | CE1 | HIS | B | 111 | 17.422 | 2.161 | 81.988 | 1.00 | 23.23 | C |
| ATOM | 2724 | NE2 | HIS | B | 111 | 16.778 | 1.651 | 83.025 | 1.00 | 23.00 | N |
| ATOM | 2725 | CD2 | HIS | B | 111 | 17.183 | 2.302 | 84.163 | 1.00 | 22.67 | C |
| ATOM | 2726 | N | LYS | B | 112 | 18.440 | 7.343 | 86.432 | 1.00 | 23.33 | N |
| ATOM | 2727 | CA | LYS | B | 112 | 18.998 | 8.219 | 87.462 | 1.00 | 24.62 | C |
| ATOM | 2728 | C | LYS | B | 112 | 19.122 | 7.579 | 88.861 | 1.00 | 25.25 | C |
| ATOM | 2729 | O | LYS | B | 112 | 20.185 | 7.649 | 89.489 | 1.00 | 25.69 | O |
| ATOM | 2730 | CB | LYS | B | 112 | 18.174 | 9.511 | 87.553 | 1.00 | 24.52 | C |
| ATOM | 2731 | N | ASP | B | 113 | 18.047 | 6.952 | 89.331 | 1.00 | 25.01 | N |
| ATOM | 2732 | CA | ASP | B | 113 | 18.010 | 6.398 | 90.682 | 1.00 | 25.77 | C |
| ATOM | 2733 | C | ASP | B | 113 | 18.918 | 5.182 | 90.876 | 1.00 | 25.63 | C |
| ATOM | 2734 | O | ASP | B | 113 | 19.302 | 4.876 | 91.999 | 1.00 | 25.32 | O |
| ATOM | 2735 | CB | ASP | B | 113 | 16.569 | 6.057 | 91.100 | 1.00 | 25.80 | C |
| ATOM | 2736 | N | ASN | B | 114 | 19.258 | 4.503 | 89.784 | 1.00 | 25.68 | N |
| ATOM | 2737 | CA | ASN | B | 114 | 20.008 | 3.250 | 89.854 | 1.00 | 25.96 | C |
| ATOM | 2738 | C | ASN | B | 114 | 21.384 | 3.254 | 89.153 | 1.00 | 25.63 | C |
| ATOM | 2739 | O | ASN | B | 114 | 21.887 | 2.186 | 88.791 | 1.00 | 26.34 | O |
| ATOM | 2740 | CB | ASN | B | 114 | 19.177 | 2.081 | 89.281 | 1.00 | 26.21 | C |
| ATOM | 2741 | CG | ASN | B | 114 | 17.848 | 1.869 | 89.996 | 1.00 | 27.41 | C |
| ATOM | 2742 | OD1 | ASN | B | 114 | 16.875 | 1.437 | 89.376 | 1.00 | 28.66 | O |
| ATOM | 2743 | ND2 | ASN | B | 114 | 17.801 | 2.151 | 91.293 | 1.00 | 28.65 | N |
| ATOM | 2744 | N | ILE | B | 115 | 21.991 | 4.421 | 88.951 | 1.00 | 24.55 | N |
| ATOM | 2745 | CA | ILE | B | 115 | 23.323 | 4.467 | 88.329 | 1.00 | 23.47 | C |
| ATOM | 2746 | C | ILE | B | 115 | 24.391 | 4.764 | 89.372 | 1.00 | 22.55 | C |
| ATOM | 2747 | O | ILE | B | 115 | 24.312 | 5.767 | 90.069 | 1.00 | 23.36 | O |
| ATOM | 2748 | CB | ILE | B | 115 | 23.385 | 5.512 | 87.180 | 1.00 | 23.35 | C |
| ATOM | 2749 | CG1 | ILE | B | 115 | 22.575 | 5.043 | 85.968 | 1.00 | 22.75 | C |
| ATOM | 2750 | CD1 | ILE | B | 115 | 22.255 | 6.152 | 84.979 | 1.00 | 20.82 | C |
| ATOM | 2751 | CG2 | ILE | B | 115 | 24.832 | 5.780 | 86.768 | 1.00 | 23.59 | C |
| ATOM | 2752 | N | GLY | B | 116 | 25.388 | 3.894 | 89.469 | 1.00 | 21.49 | N |
| ATOM | 2753 | CA | GLY | B | 116 | 26.478 | 4.089 | 90.401 | 1.00 | 20.02 | C |
| ATOM | 2754 | C | GLY | B | 116 | 27.621 | 4.913 | 89.839 | 1.00 | 19.62 | C |

FIG. 5TT

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2755 | O | GLY | B | 116 | 27.713 | 5.155 | 88.632 | 1.00 | 19.06 | O |
| ATOM | 2756 | N | SER | B | 117 | 28.508 | 5.332 | 90.733 | 1.00 | 19.01 | N |
| ATOM | 2757 | CA | SER | B | 117 | 29.662 | 6.137 | 90.368 | 1.00 | 18.71 | C |
| ATOM | 2758 | C | SER | B | 117 | 30.670 | 5.377 | 89.505 | 1.00 | 18.22 | C |
| ATOM | 2759 | O | SER | B | 117 | 31.384 | 5.986 | 88.708 | 1.00 | 18.79 | O |
| ATOM | 2760 | CB | SER | B | 117 | 30.341 | 6.693 | 91.619 | 1.00 | 18.47 | C |
| ATOM | 2761 | OG | SER | B | 117 | 30.498 | 5.686 | 92.602 | 1.00 | 19.34 | O |
| ATOM | 2762 | N | GLN | B | 118 | 30.729 | 4.059 | 89.654 | 1.00 | 18.01 | N |
| ATOM | 2763 | CA | GLN | B | 118 | 31.590 | 3.243 | 88.791 | 1.00 | 17.95 | C |
| ATOM | 2764 | C | GLN | B | 118 | 31.207 | 3.400 | 87.318 | 1.00 | 17.29 | C |
| ATOM | 2765 | O | GLN | B | 118 | 32.068 | 3.654 | 86.487 | 1.00 | 17.53 | O |
| ATOM | 2766 | CB | GLN | B | 118 | 31.573 | 1.763 | 89.188 | 1.00 | 17.74 | C |
| ATOM | 2767 | CG | GLN | B | 118 | 32.547 | 0.906 | 88.383 | 1.00 | 18.17 | C |
| ATOM | 2768 | CD | GLN | B | 118 | 34.010 | 1.238 | 88.691 | 1.00 | 20.76 | C |
| ATOM | 2769 | OE1 | GLN | B | 118 | 34.630 | 2.059 | 87.995 | 1.00 | 22.83 | O |
| ATOM | 2770 | NE2 | GLN | B | 118 | 34.562 | 0.605 | 89.722 | 1.00 | 17.47 | N |
| ATOM | 2771 | N | TYR | B | 119 | 29.920 | 3.264 | 87.016 | 1.00 | 16.46 | N |
| ATOM | 2772 | CA | TYR | B | 119 | 29.425 | 3.397 | 85.642 | 1.00 | 16.77 | C |
| ATOM | 2773 | C | TYR | B | 119 | 29.732 | 4.759 | 85.030 | 1.00 | 15.75 | C |
| ATOM | 2774 | O | TYR | B | 119 | 30.304 | 4.829 | 83.941 | 1.00 | 16.09 | O |
| ATOM | 2775 | CB | TYR | B | 119 | 27.921 | 3.087 | 85.564 | 1.00 | 17.48 | C |
| ATOM | 2776 | CG | TYR | B | 119 | 27.619 | 1.617 | 85.669 | 1.00 | 19.94 | C |
| ATOM | 2777 | CD1 | TYR | B | 119 | 27.203 | 0.893 | 84.561 | 1.00 | 22.91 | C |
| ATOM | 2778 | CE1 | TYR | B | 119 | 26.940 | -0.472 | 84.649 | 1.00 | 24.67 | C |
| ATOM | 2779 | CZ | TYR | B | 119 | 27.097 | -1.115 | 85.861 | 1.00 | 25.23 | C |
| ATOM | 2780 | OH | TYR | B | 119 | 26.841 | -2.461 | 85.965 | 1.00 | 27.73 | O |
| ATOM | 2781 | CE2 | TYR | B | 119 | 27.516 | -0.413 | 86.976 | 1.00 | 24.46 | C |
| ATOM | 2782 | CD2 | TYR | B | 119 | 27.777 | 0.939 | 86.874 | 1.00 | 22.91 | C |
| ATOM | 2783 | N | LEU | B | 120 | 29.375 | 5.831 | 85.742 | 1.00 | 14.38 | N |
| ATOM | 2784 | CA | LEU | B | 120 | 29.575 | 7.197 | 85.252 | 1.00 | 13.81 | C |
| ATOM | 2785 | C | LEU | B | 120 | 31.025 | 7.502 | 84.900 | 1.00 | 13.16 | C |
| ATOM | 2786 | O | LEU | B | 120 | 31.301 | 8.053 | 83.842 | 1.00 | 13.76 | O |
| ATOM | 2787 | CB | LEU | B | 120 | 29.052 | 8.235 | 86.253 | 1.00 | 13.58 | C |
| ATOM | 2788 | CG | LEU | B | 120 | 27.543 | 8.256 | 86.469 | 1.00 | 12.23 | C |
| ATOM | 2789 | CD1 | LEU | B | 120 | 27.223 | 8.790 | 87.859 | 1.00 | 13.28 | C |
| ATOM | 2790 | CD2 | LEU | B | 120 | 26.873 | 9.093 | 85.402 | 1.00 | 12.82 | C |
| ATOM | 2791 | N | LEU | B | 121 | 31.946 | 7.139 | 85.784 | 1.00 | 12.77 | N |
| ATOM | 2792 | CA | LEU | B | 121 | 33.357 | 7.370 | 85.526 | 1.00 | 12.25 | C |
| ATOM | 2793 | C | LEU | B | 121 | 33.882 | 6.459 | 84.411 | 1.00 | 12.37 | C |
| ATOM | 2794 | O | LEU | B | 121 | 34.667 | 6.906 | 83.581 | 1.00 | 12.42 | O |
| ATOM | 2795 | CB | LEU | B | 121 | 34.184 | 7.252 | 86.804 | 1.00 | 11.74 | C |
| ATOM | 2796 | CG | LEU | B | 121 | 33.832 | 8.229 | 87.928 | 1.00 | 11.87 | C |
| ATOM | 2797 | CD1 | LEU | B | 121 | 34.554 | 7.817 | 89.192 | 1.00 | 10.26 | C |
| ATOM | 2798 | CD2 | LEU | B | 121 | 34.176 | 9.687 | 87.578 | 1.00 | 10.60 | C |
| ATOM | 2799 | N | ASN | B | 122 | 33.417 | 5.211 | 84.378 | 1.00 | 12.67 | N |
| ATOM | 2800 | CA | ASN | B | 122 | 33.703 | 4.286 | 83.273 | 1.00 | 13.55 | C |
| ATOM | 2801 | C | ASN | B | 122 | 33.261 | 4.811 | 81.909 | 1.00 | 13.32 | C |
| ATOM | 2802 | O | ASN | B | 122 | 33.982 | 4.675 | 80.932 | 1.00 | 13.42 | O |
| ATOM | 2803 | CB | ASN | B | 122 | 33.058 | 2.920 | 83.527 | 1.00 | 14.53 | C |
| ATOM | 2804 | CG | ASN | B | 122 | 33.879 | 2.048 | 84.471 | 1.00 | 16.39 | C |
| ATOM | 2805 | OD1 | ASN | B | 122 | 33.495 | 0.913 | 84.780 | 1.00 | 18.52 | O |
| ATOM | 2806 | ND2 | ASN | B | 122 | 35.016 | 2.563 | 84.916 | 1.00 | 15.66 | N |
| ATOM | 2807 | N | TRP | B | 123 | 32.077 | 5.415 | 81.853 | 1.00 | 13.17 | N |
| ATOM | 2808 | CA | TRP | B | 123 | 31.615 | 6.080 | 80.638 | 1.00 | 13.35 | C |
| ATOM | 2809 | C | TRP | B | 123 | 32.543 | 7.216 | 80.210 | 1.00 | 13.88 | C |
| ATOM | 2810 | O | TRP | B | 123 | 32.834 | 7.347 | 79.023 | 1.00 | 14.68 | O |
| ATOM | 2811 | CB | TRP | B | 123 | 30.181 | 6.593 | 80.816 | 1.00 | 12.87 | C |
| ATOM | 2812 | CG | TRP | B | 123 | 29.177 | 5.480 | 81.010 | 1.00 | 12.55 | C |
| ATOM | 2813 | CD1 | TRP | B | 123 | 29.295 | 4.190 | 80.576 | 1.00 | 12.21 | C |
| ATOM | 2814 | NE1 | TRP | B | 123 | 28.189 | 3.462 | 80.941 | 1.00 | 13.70 | N |

FIG. 5UU

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2815 | CE2 | TRP | B | 123 | 27.330 | 4.274 | 81.634 | 1.00 | 12.77 | C |
| ATOM | 2816 | CD2 | TRP | B | 123 | 27.924 | 5.558 | 81.697 | 1.00 | 12.01 | C |
| ATOM | 2817 | CE3 | TRP | B | 123 | 27.235 | 6.585 | 82.365 | 1.00 | 11.73 | C |
| ATOM | 2818 | CZ3 | TRP | B | 123 | 25.999 | 6.304 | 82.935 | 1.00 | 12.50 | C |
| ATOM | 2819 | CH2 | TRP | B | 123 | 25.435 | 5.018 | 82.849 | 1.00 | 13.43 | C |
| ATOM | 2820 | CZ2 | TRP | B | 123 | 26.087 | 3.989 | 82.201 | 1.00 | 12.97 | C |
| ATOM | 2821 | N | CYS | B | 124 | 33.008 | 8.024 | 81.170 | 1.00 | 14.31 | N |
| ATOM | 2822 | CA | CYS | B | 124 | 33.850 | 9.186 | 80.864 | 1.00 | 14.56 | C |
| ATOM | 2823 | C | CYS | B | 124 | 35.177 | 8.737 | 80.259 | 1.00 | 14.32 | C |
| ATOM | 2824 | O | CYS | B | 124 | 35.694 | 9.373 | 79.331 | 1.00 | 14.44 | O |
| ATOM | 2825 | CB | CYS | B | 124 | 34.130 | 10.030 | 82.109 | 1.00 | 14.44 | C |
| ATOM | 2826 | SG | CYS | B | 124 | 32.699 | 10.768 | 82.912 | 1.00 | 17.76 | S |
| ATOM | 2827 | N | VAL | B | 125 | 35.723 | 7.652 | 80.806 | 1.00 | 13.63 | N |
| ATOM | 2828 | CA | VAL | B | 125 | 36.933 | 7.013 | 80.277 | 1.00 | 13.57 | C |
| ATOM | 2829 | C | VAL | B | 125 | 36.741 | 6.584 | 78.818 | 1.00 | 13.48 | C |
| ATOM | 2830 | O | VAL | B | 125 | 37.554 | 6.906 | 77.940 | 1.00 | 13.24 | O |
| ATOM | 2831 | CB | VAL | B | 125 | 37.331 | 5.773 | 81.127 | 1.00 | 13.46 | C |
| ATOM | 2832 | CG1 | VAL | B | 125 | 38.524 | 5.042 | 80.506 | 1.00 | 12.62 | C |
| ATOM | 2833 | CG2 | VAL | B | 125 | 37.656 | 6.189 | 82.572 | 1.00 | 13.17 | C |
| ATOM | 2834 | N | GLN | B | 126 | 35.644 | 5.872 | 78.579 | 1.00 | 12.88 | N |
| ATOM | 2835 | CA | GLN | B | 126 | 35.363 | 5.273 | 77.290 | 1.00 | 12.38 | C |
| ATOM | 2836 | C | GLN | B | 126 | 35.129 | 6.332 | 76.223 | 1.00 | 12.46 | C |
| ATOM | 2837 | O | GLN | B | 126 | 35.630 | 6.211 | 75.108 | 1.00 | 11.87 | O |
| ATOM | 2838 | CB | GLN | B | 126 | 34.150 | 4.361 | 77.410 | 1.00 | 12.65 | C |
| ATOM | 2839 | CG | GLN | B | 126 | 34.411 | 3.119 | 78.276 | 1.00 | 13.58 | C |
| ATOM | 2840 | CD | GLN | B | 126 | 33.153 | 2.298 | 78.502 | 1.00 | 14.00 | C |
| ATOM | 2841 | OE1 | GLN | B | 126 | 32.187 | 2.382 | 77.720 | 1.00 | 13.77 | O |
| ATOM | 2842 | NE2 | GLN | B | 126 | 33.153 | 1.508 | 79.565 | 1.00 | 12.78 | N |
| ATOM | 2843 | N | ILE | B | 127 | 34.367 | 7.372 | 76.570 | 1.00 | 11.33 | N |
| ATOM | 2844 | CA | ILE | B | 127 | 34.153 | 8.458 | 75.642 | 1.00 | 10.94 | C |
| ATOM | 2845 | C | ILE | B | 127 | 35.494 | 9.127 | 75.323 | 1.00 | 10.87 | C |
| ATOM | 2846 | O | ILE | B | 127 | 35.782 | 9.391 | 74.153 | 1.00 | 10.42 | O |
| ATOM | 2847 | CB | ILE | B | 127 | 33.097 | 9.452 | 76.180 | 1.00 | 10.86 | C |
| ATOM | 2848 | CG1 | ILE | B | 127 | 31.713 | 8.782 | 76.220 | 1.00 | 9.89 | C |
| ATOM | 2849 | CD1 | ILE | B | 127 | 30.797 | 9.311 | 77.320 | 1.00 | 8.13 | C |
| ATOM | 2850 | CG2 | ILE | B | 127 | 33.027 | 10.678 | 75.303 | 1.00 | 11.51 | C |
| ATOM | 2851 | N | ALA | B | 128 | 36.317 | 9.356 | 76.353 | 1.00 | 10.62 | N |
| ATOM | 2852 | CA | ALA | B | 128 | 37.653 | 9.929 | 76.165 | 1.00 | 11.48 | C |
| ATOM | 2853 | C | ALA | B | 128 | 38.542 | 9.041 | 75.283 | 1.00 | 11.99 | C |
| ATOM | 2854 | O | ALA | B | 128 | 39.309 | 9.554 | 74.474 | 1.00 | 11.95 | O |
| ATOM | 2855 | CB | ALA | B | 128 | 38.332 | 10.201 | 77.508 | 1.00 | 10.96 | C |
| ATOM | 2856 | N | LYS | B | 129 | 38.429 | 7.720 | 75.448 | 1.00 | 12.74 | N |
| ATOM | 2857 | CA | LYS | B | 129 | 39.118 | 6.760 | 74.589 | 1.00 | 14.11 | C |
| ATOM | 2858 | C | LYS | B | 129 | 38.634 | 6.859 | 73.141 | 1.00 | 14.67 | C |
| ATOM | 2859 | O | LYS | B | 129 | 39.446 | 6.924 | 72.207 | 1.00 | 14.41 | O |
| ATOM | 2860 | CB | LYS | B | 129 | 38.920 | 5.337 | 75.101 | 1.00 | 14.55 | C |
| ATOM | 2861 | CG | LYS | B | 129 | 39.789 | 4.989 | 76.285 | 1.00 | 15.79 | C |
| ATOM | 2862 | CD | LYS | B | 129 | 39.633 | 3.531 | 76.668 | 1.00 | 17.46 | C |
| ATOM | 2863 | CE | LYS | B | 129 | 40.681 | 3.153 | 77.693 | 1.00 | 18.76 | C |
| ATOM | 2864 | NZ | LYS | B | 129 | 40.137 | 2.204 | 78.705 | 1.00 | 21.51 | N |
| ATOM | 2865 | N | GLY | B | 130 | 37.313 | 6.884 | 72.960 | 1.00 | 14.43 | N |
| ATOM | 2866 | CA | GLY | B | 130 | 36.737 | 7.005 | 71.629 | 1.00 | 15.01 | C |
| ATOM | 2867 | C | GLY | B | 130 | 37.220 | 8.250 | 70.901 | 1.00 | 14.80 | C |
| ATOM | 2868 | O | GLY | B | 130 | 37.609 | 8.198 | 69.741 | 1.00 | 15.09 | O |
| ATOM | 2869 | N | MET | B | 131 | 37.211 | 9.369 | 71.612 | 1.00 | 15.03 | N |
| ATOM | 2870 | CA | MET | B | 131 | 37.609 | 10.673 | 71.075 | 1.00 | 14.67 | C |
| ATOM | 2871 | C | MET | B | 131 | 39.104 | 10.782 | 70.773 | 1.00 | 14.50 | C |
| ATOM | 2872 | O | MET | B | 131 | 39.495 | 11.451 | 69.821 | 1.00 | 13.93 | O |
| ATOM | 2873 | CB | MET | B | 131 | 37.208 | 11.774 | 72.065 | 1.00 | 14.52 | C |
| ATOM | 2874 | CG | MET | B | 131 | 35.717 | 12.074 | 72.121 | 1.00 | 13.78 | C |

FIG. 5VV

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2875 | SD | MET | B | 131 | 34.940 | 12.339 | 70.502 | 1.00 | 14.79 | S |
| ATOM | 2876 | CE | MET | B | 131 | 35.858 | 13.687 | 69.878 | 1.00 | 16.01 | C |
| ATOM | 2877 | N | ASN | B | 132 | 39.919 | 10.125 | 71.599 | 1.00 | 15.17 | N |
| ATOM | 2878 | CA | ASN | B | 132 | 41.367 | 10.057 | 71.420 | 1.00 | 15.77 | C |
| ATOM | 2879 | C | ASN | B | 132 | 41.741 | 9.276 | 70.173 | 1.00 | 16.20 | C |
| ATOM | 2880 | O | ASN | B | 132 | 42.738 | 9.594 | 69.510 | 1.00 | 16.12 | O |
| ATOM | 2881 | CB | ASN | B | 132 | 42.038 | 9.428 | 72.656 | 1.00 | 15.64 | C |
| ATOM | 2882 | CG | ASN | B | 132 | 43.550 | 9.258 | 72.495 | 1.00 | 16.46 | C |
| ATOM | 2883 | OD1 | ASN | B | 132 | 44.280 | 10.222 | 72.251 | 1.00 | 16.30 | O |
| ATOM | 2884 | ND2 | ASN | B | 132 | 44.023 | 8.020 | 72.638 | 1.00 | 17.97 | N |
| ATOM | 2885 | N | TYR | B | 133 | 40.948 | 8.247 | 69.869 | 1.00 | 16.69 | N |
| ATOM | 2886 | CA | TYR | B | 133 | 41.097 | 7.510 | 68.614 | 1.00 | 17.96 | C |
| ATOM | 2887 | C | TYR | B | 133 | 40.856 | 8.438 | 67.432 | 1.00 | 18.55 | C |
| ATOM | 2888 | O | TYR | B | 133 | 41.637 | 8.458 | 66.483 | 1.00 | 18.74 | O |
| ATOM | 2889 | CB | TYR | B | 133 | 40.140 | 6.321 | 68.547 | 1.00 | 17.70 | C |
| ATOM | 2890 | CG | TYR | B | 133 | 40.045 | 5.704 | 67.171 | 1.00 | 18.47 | C |
| ATOM | 2891 | CD1 | TYR | B | 133 | 40.994 | 4.769 | 66.732 | 1.00 | 18.22 | C |
| ATOM | 2892 | CE1 | TYR | B | 133 | 40.906 | 4.200 | 65.464 | 1.00 | 17.82 | C |
| ATOM | 2893 | CZ | TYR | B | 133 | 39.860 | 4.560 | 64.624 | 1.00 | 17.71 | C |
| ATOM | 2894 | OH | TYR | B | 133 | 39.766 | 4.007 | 63.377 | 1.00 | 18.07 | O |
| ATOM | 2895 | CE2 | TYR | B | 133 | 38.918 | 5.483 | 65.025 | 1.00 | 17.89 | C |
| ATOM | 2896 | CD2 | TYR | B | 133 | 39.011 | 6.053 | 66.300 | 1.00 | 18.32 | C |
| ATOM | 2897 | N | LEU | B | 134 | 39.773 | 9.210 | 67.504 | 1.00 | 19.23 | N |
| ATOM | 2898 | CA | LEU | B | 134 | 39.438 | 10.159 | 66.449 | 1.00 | 19.76 | C |
| ATOM | 2899 | C | LEU | B | 134 | 40.540 | 11.195 | 66.282 | 1.00 | 19.69 | C |
| ATOM | 2900 | O | LEU | B | 134 | 40.894 | 11.543 | 65.156 | 1.00 | 19.19 | O |
| ATOM | 2901 | CB | LEU | B | 134 | 38.092 | 10.840 | 66.723 | 1.00 | 19.86 | C |
| ATOM | 2902 | CG | LEU | B | 134 | 36.800 | 10.015 | 66.639 | 1.00 | 20.31 | C |
| ATOM | 2903 | CD1 | LEU | B | 134 | 35.606 | 10.936 | 66.854 | 1.00 | 21.10 | C |
| ATOM | 2904 | CD2 | LEU | B | 134 | 36.656 | 9.272 | 65.318 | 1.00 | 20.78 | C |
| ATOM | 2905 | N | GLU | B | 135 | 41.091 | 11.672 | 67.402 | 1.00 | 20.10 | N |
| ATOM | 2906 | CA | GLU | B | 135 | 42.221 | 12.598 | 67.347 | 1.00 | 20.27 | C |
| ATOM | 2907 | C | GLU | B | 135 | 43.437 | 11.965 | 66.678 | 1.00 | 20.05 | C |
| ATOM | 2908 | O | GLU | B | 135 | 44.058 | 12.592 | 65.832 | 1.00 | 20.59 | O |
| ATOM | 2909 | CB | GLU | B | 135 | 42.587 | 13.161 | 68.721 | 1.00 | 20.54 | C |
| ATOM | 2910 | CG | GLU | B | 135 | 43.786 | 14.109 | 68.667 | 1.00 | 21.54 | C |
| ATOM | 2911 | CD | GLU | B | 135 | 44.085 | 14.812 | 69.982 | 1.00 | 22.97 | C |
| ATOM | 2912 | OE1 | GLU | B | 135 | 43.412 | 14.526 | 71.000 | 1.00 | 22.28 | O |
| ATOM | 2913 | OE2 | GLU | B | 135 | 45.009 | 15.656 | 69.990 | 1.00 | 22.62 | O |
| ATOM | 2914 | N | ASP | B | 136 | 43.756 | 10.726 | 67.046 | 1.00 | 19.95 | N |
| ATOM | 2915 | CA | ASP | B | 136 | 44.869 | 9.997 | 66.449 | 1.00 | 20.02 | C |
| ATOM | 2916 | C | ASP | B | 136 | 44.740 | 9.871 | 64.941 | 1.00 | 20.16 | C |
| ATOM | 2917 | O | ASP | B | 136 | 45.741 | 9.952 | 64.226 | 1.00 | 20.42 | O |
| ATOM | 2918 | CB | ASP | B | 136 | 44.994 | 8.608 | 67.050 | 1.00 | 20.30 | C |
| ATOM | 2919 | CG | ASP | B | 136 | 45.727 | 8.607 | 68.368 | 1.00 | 20.85 | C |
| ATOM | 2920 | OD1 | ASP | B | 136 | 45.631 | 7.578 | 69.065 | 1.00 | 21.59 | O |
| ATOM | 2921 | OD2 | ASP | B | 136 | 46.418 | 9.567 | 68.785 | 1.00 | 20.39 | O |
| ATOM | 2922 | N | ARG | B | 137 | 43.503 | 9.679 | 64.479 | 1.00 | 20.00 | N |
| ATOM | 2923 | CA | ARG | B | 137 | 43.161 | 9.639 | 63.058 | 1.00 | 19.04 | C |
| ATOM | 2924 | C | ARG | B | 137 | 43.007 | 11.041 | 62.468 | 1.00 | 18.83 | C |
| ATOM | 2925 | O | ARG | B | 137 | 42.636 | 11.196 | 61.298 | 1.00 | 18.70 | O |
| ATOM | 2926 | CB | ARG | B | 137 | 41.860 | 8.859 | 62.862 | 1.00 | 19.57 | C |
| ATOM | 2927 | CG | ARG | B | 137 | 42.013 | 7.337 | 62.920 | 1.00 | 21.49 | C |
| ATOM | 2928 | CD | ARG | B | 137 | 42.519 | 6.715 | 61.616 | 1.00 | 24.05 | C |
| ATOM | 2929 | NE | ARG | B | 137 | 41.420 | 6.330 | 60.730 | 1.00 | 27.27 | N |
| ATOM | 2930 | CZ | ARG | B | 137 | 40.949 | 7.083 | 59.745 | 1.00 | 28.83 | C |
| ATOM | 2931 | NH1 | ARG | B | 137 | 41.473 | 8.278 | 59.498 | 1.00 | 32.73 | N |
| ATOM | 2932 | NH2 | ARG | B | 137 | 39.960 | 6.643 | 58.991 | 1.00 | 28.41 | N |
| ATOM | 2933 | N | ARG | B | 138 | 43.285 | 12.061 | 63.280 | 1.00 | 18.28 | N |
| ATOM | 2934 | CA | ARG | B | 138 | 43.136 | 13.457 | 62.866 | 1.00 | 18.11 | C |

FIG. 5WW

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2935 | C | ARG | B | 138 | 41.753 | 13.696 | 62.265 | 1.00 | 18.18 | C |
| ATOM | 2936 | O | ARG | B | 138 | 41.599 | 14.375 | 61.245 | 1.00 | 18.83 | O |
| ATOM | 2937 | CB | ARG | B | 138 | 44.260 | 13.886 | 61.907 | 1.00 | 18.64 | C |
| ATOM | 2938 | N | LEU | B | 139 | 40.748 | 13.112 | 62.909 | 1.00 | 17.18 | N |
| ATOM | 2939 | CA | LEU | B | 139 | 39.364 | 13.363 | 62.564 | 1.00 | 16.85 | C |
| ATOM | 2940 | C | LEU | B | 139 | 38.742 | 14.200 | 63.695 | 1.00 | 16.74 | C |
| ATOM | 2941 | O | LEU | B | 139 | 38.939 | 13.915 | 64.888 | 1.00 | 16.86 | O |
| ATOM | 2942 | CB | LEU | B | 139 | 38.606 | 12.042 | 62.343 | 1.00 | 16.37 | C |
| ATOM | 2943 | CG | LEU | B | 139 | 39.128 | 11.058 | 61.275 | 1.00 | 16.51 | C |
| ATOM | 2944 | CD1 | LEU | B | 139 | 38.504 | 9.657 | 61.383 | 1.00 | 13.92 | C |
| ATOM | 2945 | CD2 | LEU | B | 139 | 38.946 | 11.626 | 59.857 | 1.00 | 17.30 | C |
| ATOM | 2946 | N | VAL | B | 140 | 38.023 | 15.247 | 63.317 | 1.00 | 16.28 | N |
| ATOM | 2947 | CA | VAL | B | 140 | 37.331 | 16.094 | 64.280 | 1.00 | 16.21 | C |
| ATOM | 2948 | C | VAL | B | 140 | 35.846 | 15.702 | 64.276 | 1.00 | 16.75 | C |
| ATOM | 2949 | O | VAL | B | 140 | 35.207 | 15.662 | 63.217 | 1.00 | 16.46 | O |
| ATOM | 2950 | CB | VAL | B | 140 | 37.542 | 17.598 | 63.949 | 1.00 | 16.72 | C |
| ATOM | 2951 | CG1 | VAL | B | 140 | 36.636 | 18.499 | 64.817 | 1.00 | 16.04 | C |
| ATOM | 2952 | CG2 | VAL | B | 140 | 39.055 | 17.998 | 64.089 | 1.00 | 14.20 | C |
| ATOM | 2953 | N | HIS | B | 141 | 35.305 | 15.387 | 65.453 | 1.00 | 17.21 | N |
| ATOM | 2954 | CA | HIS | B | 141 | 33.905 | 14.984 | 65.552 | 1.00 | 17.28 | C |
| ATOM | 2955 | C | HIS | B | 141 | 32.964 | 16.159 | 65.378 | 1.00 | 17.55 | C |
| ATOM | 2956 | O | HIS | B | 141 | 32.042 | 16.084 | 64.563 | 1.00 | 17.43 | O |
| ATOM | 2957 | CB | HIS | B | 141 | 33.598 | 14.248 | 66.860 | 1.00 | 17.34 | C |
| ATOM | 2958 | CG | HIS | B | 141 | 32.215 | 13.672 | 66.905 | 1.00 | 17.38 | C |
| ATOM | 2959 | ND1 | HIS | B | 141 | 31.081 | 14.458 | 66.950 | 1.00 | 17.18 | N |
| ATOM | 2960 | CE1 | HIS | B | 141 | 30.011 | 13.683 | 66.969 | 1.00 | 17.34 | C |
| ATOM | 2961 | NE2 | HIS | B | 141 | 30.408 | 12.424 | 66.933 | 1.00 | 16.82 | N |
| ATOM | 2962 | CD2 | HIS | B | 141 | 31.781 | 12.390 | 66.885 | 1.00 | 17.27 | C |
| ATOM | 2963 | N | ARG | B | 142 | 33.171 | 17.214 | 66.175 | 1.00 | 17.67 | N |
| ATOM | 2964 | CA | ARG | B | 142 | 32.470 | 18.491 | 66.000 | 1.00 | 18.29 | C |
| ATOM | 2965 | C | ARG | B | 142 | 31.061 | 18.558 | 66.626 | 1.00 | 18.17 | C |
| ATOM | 2966 | O | ARG | B | 142 | 30.499 | 19.643 | 66.791 | 1.00 | 18.43 | O |
| ATOM | 2967 | CB | ARG | B | 142 | 32.468 | 18.854 | 64.506 | 1.00 | 19.02 | C |
| ATOM | 2968 | CG | ARG | B | 142 | 31.723 | 20.091 | 64.097 | 1.00 | 21.75 | C |
| ATOM | 2969 | CD | ARG | B | 142 | 31.557 | 20.214 | 62.586 | 1.00 | 25.73 | C |
| ATOM | 2970 | NE | ARG | B | 142 | 32.837 | 20.240 | 61.876 | 1.00 | 27.56 | N |
| ATOM | 2971 | CZ | ARG | B | 142 | 33.180 | 21.185 | 61.008 | 1.00 | 29.58 | C |
| ATOM | 2972 | NH1 | ARG | B | 142 | 32.337 | 22.187 | 60.744 | 1.00 | 30.12 | N |
| ATOM | 2973 | NH2 | ARG | B | 142 | 34.360 | 21.135 | 60.402 | 1.00 | 28.92 | N |
| ATOM | 2974 | N | ASP | B | 143 | 30.495 | 17.414 | 66.996 | 1.00 | 17.99 | N |
| ATOM | 2975 | CA | ASP | B | 143 | 29.174 | 17.404 | 67.624 | 1.00 | 18.25 | C |
| ATOM | 2976 | C | ASP | B | 143 | 29.074 | 16.409 | 68.781 | 1.00 | 17.20 | C |
| ATOM | 2977 | O | ASP | B | 143 | 28.086 | 15.690 | 68.902 | 1.00 | 16.71 | O |
| ATOM | 2978 | CB | ASP | B | 143 | 28.082 | 17.135 | 66.574 | 1.00 | 19.03 | C |
| ATOM | 2979 | CG | ASP | B | 143 | 26.679 | 17.479 | 67.062 | 1.00 | 20.93 | C |
| ATOM | 2980 | OD1 | ASP | B | 143 | 26.511 | 18.036 | 68.179 | 1.00 | 20.76 | O |
| ATOM | 2981 | OD2 | ASP | B | 143 | 25.665 | 17.228 | 66.365 | 1.00 | 24.70 | O |
| ATOM | 2982 | N | LEU | B | 144 | 30.093 | 16.383 | 69.637 | 1.00 | 16.54 | N |
| ATOM | 2983 | CA | LEU | B | 144 | 30.066 | 15.517 | 70.814 | 1.00 | 15.72 | C |
| ATOM | 2984 | C | LEU | B | 144 | 29.096 | 16.081 | 71.866 | 1.00 | 15.06 | C |
| ATOM | 2985 | O | LEU | B | 144 | 29.178 | 17.257 | 72.243 | 1.00 | 14.74 | O |
| ATOM | 2986 | CB | LEU | B | 144 | 31.477 | 15.329 | 71.394 | 1.00 | 15.69 | C |
| ATOM | 2987 | CG | LEU | B | 144 | 31.643 | 14.508 | 72.680 | 1.00 | 16.01 | C |
| ATOM | 2988 | CD1 | LEU | B | 144 | 31.310 | 13.046 | 72.448 | 1.00 | 16.11 | C |
| ATOM | 2989 | CD2 | LEU | B | 144 | 33.061 | 14.634 | 73.200 | 1.00 | 16.80 | C |
| ATOM | 2990 | N | ALA | B | 145 | 28.168 | 15.226 | 72.292 | 1.00 | 14.04 | N |
| ATOM | 2991 | CA | ALA | B | 145 | 27.172 | 15.517 | 73.332 | 1.00 | 13.13 | C |
| ATOM | 2992 | C | ALA | B | 145 | 26.646 | 14.179 | 73.840 | 1.00 | 12.94 | C |
| ATOM | 2993 | O | ALA | B | 145 | 26.835 | 13.149 | 73.183 | 1.00 | 12.84 | O |
| ATOM | 2994 | CB | ALA | B | 145 | 26.024 | 16.361 | 72.775 | 1.00 | 12.20 | C |

FIG. 5XX

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2995 | N | ALA | B | 146 | 25.982 | 14.183 | 74.996 | 1.00 | 12.87 | N |
| ATOM | 2996 | CA | ALA | B | 146 | 25.345 | 12.969 | 75.496 | 1.00 | 13.05 | C |
| ATOM | 2997 | C | ALA | B | 146 | 24.318 | 12.367 | 74.514 | 1.00 | 13.32 | C |
| ATOM | 2998 | O | ALA | B | 146 | 24.165 | 11.147 | 74.455 | 1.00 | 13.18 | O |
| ATOM | 2999 | CB | ALA | B | 146 | 24.723 | 13.205 | 76.867 | 1.00 | 12.55 | C |
| ATOM | 3000 | N | ARG | B | 147 | 23.620 | 13.215 | 73.754 | 1.00 | 13.75 | N |
| ATOM | 3001 | CA | ARG | B | 147 | 22.671 | 12.742 | 72.730 | 1.00 | 15.11 | C |
| ATOM | 3002 | C | ARG | B | 147 | 23.342 | 11.909 | 71.642 | 1.00 | 15.27 | C |
| ATOM | 3003 | O | ARG | B | 147 | 22.711 | 11.061 | 71.022 | 1.00 | 16.36 | O |
| ATOM | 3004 | CB | ARG | B | 147 | 21.888 | 13.907 | 72.098 | 1.00 | 15.25 | C |
| ATOM | 3005 | CG | ARG | B | 147 | 22.692 | 14.779 | 71.128 | 1.00 | 16.01 | C |
| ATOM | 3006 | CD | ARG | B | 147 | 21.951 | 16.033 | 70.657 | 1.00 | 15.00 | C |
| ATOM | 3007 | NE | ARG | B | 147 | 22.881 | 17.005 | 70.105 | 1.00 | 15.92 | N |
| ATOM | 3008 | CZ | ARG | B | 147 | 23.429 | 18.008 | 70.792 | 1.00 | 15.52 | C |
| ATOM | 3009 | NH1 | ARG | B | 147 | 23.138 | 18.207 | 72.070 | 1.00 | 14.10 | N |
| ATOM | 3010 | NH2 | ARG | B | 147 | 24.266 | 18.827 | 70.184 | 1.00 | 17.23 | N |
| ATOM | 3011 | N | ASN | B | 148 | 24.633 | 12.139 | 71.434 | 1.00 | 16.22 | N |
| ATOM | 3012 | CA | ASN | B | 148 | 25.398 | 11.423 | 70.417 | 1.00 | 16.00 | C |
| ATOM | 3013 | C | ASN | B | 148 | 26.327 | 10.372 | 70.993 | 1.00 | 15.46 | C |
| ATOM | 3014 | O | ASN | B | 148 | 27.364 | 10.065 | 70.405 | 1.00 | 14.79 | O |
| ATOM | 3015 | CB | ASN | B | 148 | 26.155 | 12.421 | 69.539 | 1.00 | 16.57 | C |
| ATOM | 3016 | CG | ASN | B | 148 | 25.218 | 13.279 | 68.717 | 1.00 | 17.29 | C |
| ATOM | 3017 | OD1 | ASN | B | 148 | 25.352 | 14.499 | 68.674 | 1.00 | 18.79 | O |
| ATOM | 3018 | ND2 | ASN | B | 148 | 24.247 | 12.641 | 68.072 | 1.00 | 17.30 | N |
| ATOM | 3019 | N | VAL | B | 149 | 25.952 | 9.839 | 72.158 | 1.00 | 15.09 | N |
| ATOM | 3020 | CA | VAL | B | 149 | 26.628 | 8.675 | 72.729 | 1.00 | 14.53 | C |
| ATOM | 3021 | C | VAL | B | 149 | 25.581 | 7.595 | 72.925 | 1.00 | 14.66 | C |
| ATOM | 3022 | O | VAL | B | 149 | 24.496 | 7.859 | 73.436 | 1.00 | 15.29 | O |
| ATOM | 3023 | CB | VAL | B | 149 | 27.372 | 8.995 | 74.056 | 1.00 | 14.48 | C |
| ATOM | 3024 | CG1 | VAL | B | 149 | 28.010 | 7.749 | 74.644 | 1.00 | 14.28 | C |
| ATOM | 3025 | CG2 | VAL | B | 149 | 28.449 | 10.061 | 73.842 | 1.00 | 13.23 | C |
| ATOM | 3026 | N | LEU | B | 150 | 25.896 | 6.386 | 72.479 | 1.00 | 15.22 | N |
| ATOM | 3027 | CA | LEU | B | 150 | 24.958 | 5.270 | 72.537 | 1.00 | 14.96 | C |
| ATOM | 3028 | C | LEU | B | 150 | 25.418 | 4.214 | 73.514 | 1.00 | 15.33 | C |
| ATOM | 3029 | O | LEU | B | 150 | 26.604 | 4.108 | 73.816 | 1.00 | 15.82 | O |
| ATOM | 3030 | CB | LEU | B | 150 | 24.756 | 4.654 | 71.150 | 1.00 | 13.86 | C |
| ATOM | 3031 | CG | LEU | B | 150 | 24.285 | 5.582 | 70.025 | 1.00 | 14.68 | C |
| ATOM | 3032 | CD1 | LEU | B | 150 | 24.130 | 4.811 | 68.707 | 1.00 | 13.79 | C |
| ATOM | 3033 | CD2 | LEU | B | 150 | 22.992 | 6.348 | 70.375 | 1.00 | 13.31 | C |
| ATOM | 3034 | N | VAL | B | 151 | 24.460 | 3.423 | 73.982 | 1.00 | 16.46 | N |
| ATOM | 3035 | CA | VAL | B | 151 | 24.675 | 2.401 | 74.999 | 1.00 | 17.20 | C |
| ATOM | 3036 | C | VAL | B | 151 | 24.583 | 1.004 | 74.372 | 1.00 | 17.68 | C |
| ATOM | 3037 | O | VAL | B | 151 | 23.496 | 0.543 | 74.042 | 1.00 | 18.67 | O |
| ATOM | 3038 | CB | VAL | B | 151 | 23.629 | 2.540 | 76.139 | 1.00 | 17.11 | C |
| ATOM | 3039 | CG1 | VAL | B | 151 | 23.949 | 1.615 | 77.315 | 1.00 | 18.23 | C |
| ATOM | 3040 | CG2 | VAL | B | 151 | 23.528 | 3.980 | 76.619 | 1.00 | 16.48 | C |
| ATOM | 3041 | N | LYS | B | 152 | 25.731 | 0.352 | 74.196 | 1.00 | 18.57 | N |
| ATOM | 3042 | CA | LYS | B | 152 | 25.800 | -1.036 | 73.734 | 1.00 | 18.95 | C |
| ATOM | 3043 | C | LYS | B | 152 | 25.396 | -1.967 | 74.868 | 1.00 | 19.76 | C |
| ATOM | 3044 | O | LYS | B | 152 | 24.471 | -2.768 | 74.730 | 1.00 | 19.89 | O |
| ATOM | 3045 | CB | LYS | B | 152 | 27.217 | -1.365 | 73.252 | 1.00 | 19.11 | C |
| ATOM | 3046 | CG | LYS | B | 152 | 27.360 | -2.726 | 72.575 | 1.00 | 19.33 | C |
| ATOM | 3047 | N | THR | B | 153 | 26.117 | -1.873 | 75.983 | 1.00 | 20.44 | N |
| ATOM | 3048 | CA | THR | B | 153 | 25.679 | -2.475 | 77.244 | 1.00 | 21.72 | C |
| ATOM | 3049 | C | THR | B | 153 | 25.777 | -1.359 | 78.262 | 1.00 | 21.90 | C |
| ATOM | 3050 | O | THR | B | 153 | 26.413 | -0.348 | 77.981 | 1.00 | 22.30 | O |
| ATOM | 3051 | CB | THR | B | 153 | 26.555 | -3.692 | 77.659 | 1.00 | 21.38 | C |
| ATOM | 3052 | OG1 | THR | B | 153 | 27.840 | -3.236 | 78.095 | 1.00 | 21.96 | O |
| ATOM | 3053 | CG2 | THR | B | 153 | 26.870 | -4.593 | 76.455 | 1.00 | 20.61 | C |
| ATOM | 3054 | N | PRO | B | 154 | 25.123 | -1.506 | 79.413 | 1.00 | 22.82 | N |

FIG. 5YY

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3055 | CA | PRO | B | 154 | 25.261 | -0.537 | 80.508 | 1.00 | 23.06 | C |
| ATOM | 3056 | C | PRO | B | 154 | 26.712 | -0.201 | 80.870 | 1.00 | 23.28 | C |
| ATOM | 3057 | O | PRO | B | 154 | 26.952 | 0.855 | 81.442 | 1.00 | 23.52 | O |
| ATOM | 3058 | CB | PRO | B | 154 | 24.567 | -1.246 | 81.670 | 1.00 | 23.42 | C |
| ATOM | 3059 | CG | PRO | B | 154 | 23.496 | -2.025 | 81.012 | 1.00 | 22.85 | C |
| ATOM | 3060 | CD | PRO | B | 154 | 24.157 | -2.569 | 79.757 | 1.00 | 23.16 | C |
| ATOM | 3061 | N | GLN | B | 155 | 27.662 | -1.065 | 80.536 | 1.00 | 23.65 | N |
| ATOM | 3062 | CA | GLN | B | 155 | 29.065 | -0.768 | 80.825 | 1.00 | 24.53 | C |
| ATOM | 3063 | C | GLN | B | 155 | 29.938 | -0.624 | 79.571 | 1.00 | 23.64 | C |
| ATOM | 3064 | O | GLN | B | 155 | 31.161 | -0.693 | 79.648 | 1.00 | 24.23 | O |
| ATOM | 3065 | CB | GLN | B | 155 | 29.652 | -1.797 | 81.802 | 1.00 | 25.66 | C |
| ATOM | 3066 | CG | GLN | B | 155 | 29.604 | -3.224 | 81.294 | 1.00 | 28.59 | C |
| ATOM | 3067 | CD | GLN | B | 155 | 28.726 | -4.107 | 82.147 | 1.00 | 31.84 | C |
| ATOM | 3068 | OE1 | GLN | B | 155 | 27.497 | -4.115 | 81.999 | 1.00 | 34.01 | O |
| ATOM | 3069 | NE2 | GLN | B | 155 | 29.347 | -4.860 | 83.041 | 1.00 | 32.93 | N |
| ATOM | 3070 | N | HIS | B | 156 | 29.301 | -0.400 | 78.426 | 1.00 | 22.82 | N |
| ATOM | 3071 | CA | HIS | B | 156 | 30.010 | -0.202 | 77.169 | 1.00 | 22.02 | C |
| ATOM | 3072 | C | HIS | B | 156 | 29.281 | 0.829 | 76.307 | 1.00 | 21.21 | C |
| ATOM | 3073 | O | HIS | B | 156 | 28.208 | 0.560 | 75.788 | 1.00 | 21.40 | O |
| ATOM | 3074 | CB | HIS | B | 156 | 30.182 | -1.537 | 76.428 | 1.00 | 21.76 | C |
| ATOM | 3075 | CG | HIS | B | 156 | 30.984 | -1.442 | 75.162 | 1.00 | 22.91 | C |
| ATOM | 3076 | ND1 | HIS | B | 156 | 31.532 | -0.263 | 74.705 | 1.00 | 22.28 | N |
| ATOM | 3077 | CE1 | HIS | B | 156 | 32.168 | -0.483 | 73.570 | 1.00 | 21.49 | C |
| ATOM | 3078 | NE2 | HIS | B | 156 | 32.059 | -1.764 | 73.273 | 1.00 | 22.52 | N |
| ATOM | 3079 | CD2 | HIS | B | 156 | 31.322 | -2.387 | 74.251 | 1.00 | 23.10 | C |
| ATOM | 3080 | N | VAL | B | 157 | 29.879 | 2.011 | 76.160 | 1.00 | 20.75 | N |
| ATOM | 3081 | CA | VAL | B | 157 | 29.285 | 3.081 | 75.362 | 1.00 | 19.33 | C |
| ATOM | 3082 | C | VAL | B | 157 | 30.135 | 3.428 | 74.141 | 1.00 | 19.44 | C |
| ATOM | 3083 | O | VAL | B | 157 | 31.324 | 3.095 | 74.083 | 1.00 | 19.26 | O |
| ATOM | 3084 | CB | VAL | B | 157 | 28.955 | 4.358 | 76.209 | 1.00 | 19.85 | C |
| ATOM | 3085 | CG1 | VAL | B | 157 | 27.941 | 4.029 | 77.327 | 1.00 | 18.01 | C |
| ATOM | 3086 | CG2 | VAL | B | 157 | 30.230 | 5.038 | 76.763 | 1.00 | 17.58 | C |
| ATOM | 3087 | N | LYS | B | 158 | 29.506 | 4.103 | 73.177 | 1.00 | 19.20 | N |
| ATOM | 3088 | CA | LYS | B | 158 | 30.088 | 4.375 | 71.864 | 1.00 | 18.62 | C |
| ATOM | 3089 | C | LYS | B | 158 | 29.623 | 5.725 | 71.326 | 1.00 | 18.34 | C |
| ATOM | 3090 | O | LYS | B | 158 | 28.429 | 6.060 | 71.392 | 1.00 | 17.75 | O |
| ATOM | 3091 | CB | LYS | B | 158 | 29.646 | 3.292 | 70.876 | 1.00 | 18.95 | C |
| ATOM | 3092 | CG | LYS | B | 158 | 30.759 | 2.430 | 70.330 | 1.00 | 20.37 | C |
| ATOM | 3093 | CD | LYS | B | 158 | 30.330 | 0.978 | 70.248 | 1.00 | 21.15 | C |
| ATOM | 3094 | CE | LYS | B | 158 | 30.359 | 0.490 | 68.827 | 1.00 | 22.24 | C |
| ATOM | 3095 | NZ | LYS | B | 158 | 31.698 | -0.008 | 68.384 | 1.00 | 24.66 | N |
| ATOM | 3096 | N | ILE | B | 159 | 30.562 | 6.481 | 70.770 | 1.00 | 17.82 | N |
| ATOM | 3097 | CA | ILE | B | 159 | 30.259 | 7.758 | 70.147 | 1.00 | 18.47 | C |
| ATOM | 3098 | C | ILE | B | 159 | 29.677 | 7.522 | 68.761 | 1.00 | 18.97 | C |
| ATOM | 3099 | O | ILE | B | 159 | 30.229 | 6.770 | 67.950 | 1.00 | 19.06 | O |
| ATOM | 3100 | CB | ILE | B | 159 | 31.524 | 8.654 | 70.082 | 1.00 | 18.12 | C |
| ATOM | 3101 | CG1 | ILE | B | 159 | 31.978 | 9.028 | 71.491 | 1.00 | 18.56 | C |
| ATOM | 3102 | CD1 | ILE | B | 159 | 33.479 | 8.986 | 71.658 | 1.00 | 21.02 | C |
| ATOM | 3103 | CG2 | ILE | B | 159 | 31.267 | 9.926 | 69.289 | 1.00 | 16.71 | C |
| ATOM | 3104 | N | THR | B | 160 | 28.556 | 8.171 | 68.491 | 1.00 | 19.88 | N |
| ATOM | 3105 | CA | THR | B | 160 | 27.917 | 8.051 | 67.193 | 1.00 | 20.98 | C |
| ATOM | 3106 | C | THR | B | 160 | 27.820 | 9.407 | 66.487 | 1.00 | 22.04 | C |
| ATOM | 3107 | O | THR | B | 160 | 28.242 | 10.431 | 67.038 | 1.00 | 21.56 | O |
| ATOM | 3108 | CB | THR | B | 160 | 26.550 | 7.358 | 67.345 | 1.00 | 20.81 | C |
| ATOM | 3109 | OG1 | THR | B | 160 | 26.034 | 7.011 | 66.055 | 1.00 | 21.04 | O |
| ATOM | 3110 | CG2 | THR | B | 160 | 25.507 | 8.315 | 67.906 | 1.00 | 21.77 | C |
| ATOM | 3111 | N | ASP | B | 161 | 27.312 | 9.380 | 65.251 | 1.00 | 23.57 | N |
| ATOM | 3112 | CA | ASP | B | 161 | 26.982 | 10.564 | 64.452 | 1.00 | 25.46 | C |
| ATOM | 3113 | C | ASP | B | 161 | 28.185 | 11.368 | 63.951 | 1.00 | 25.96 | C |
| ATOM | 3114 | O | ASP | B | 161 | 28.025 | 12.494 | 63.468 | 1.00 | 25.51 | O |

FIG. 5ZZ

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3115 | CB | ASP | B | 161 | 25.965 | 11.474 | 65.178 | 1.00 | 25.64 | C |
| ATOM | 3116 | CG | ASP | B | 161 | 24.518 | 11.006 | 64.995 | 1.00 | 27.57 | C |
| ATOM | 3117 | OD1 | ASP | B | 161 | 24.306 | 9.900 | 64.456 | 1.00 | 27.77 | O |
| ATOM | 3118 | OD2 | ASP | B | 161 | 23.523 | 11.676 | 65.359 | 1.00 | 28.44 | O |
| ATOM | 3119 | N | PHE | B | 162 | 29.382 | 10.804 | 64.044 | 1.00 | 27.00 | N |
| ATOM | 3120 | CA | PHE | B | 162 | 30.544 | 11.501 | 63.497 | 1.00 | 28.97 | C |
| ATOM | 3121 | C | PHE | B | 162 | 30.435 | 11.591 | 61.968 | 1.00 | 29.91 | C |
| ATOM | 3122 | O | PHE | B | 162 | 30.004 | 10.635 | 61.304 | 1.00 | 29.51 | O |
| ATOM | 3123 | CB | PHE | B | 162 | 31.856 | 10.854 | 63.947 | 1.00 | 29.25 | C |
| ATOM | 3124 | CG | PHE | B | 162 | 32.403 | 9.882 | 62.975 | 1.00 | 30.69 | C |
| ATOM | 3125 | CD1 | PHE | B | 162 | 31.964 | 8.564 | 62.983 | 1.00 | 32.77 | C |
| ATOM | 3126 | CE1 | PHE | B | 162 | 32.443 | 7.661 | 62.069 | 1.00 | 32.93 | C |
| ATOM | 3127 | CZ | PHE | B | 162 | 33.389 | 8.085 | 61.139 | 1.00 | 33.64 | C |
| ATOM | 3128 | CE2 | PHE | B | 162 | 33.823 | 9.403 | 61.114 | 1.00 | 31.87 | C |
| ATOM | 3129 | CD2 | PHE | B | 162 | 33.334 | 10.286 | 62.029 | 1.00 | 31.34 | C |
| ATOM | 3130 | N | GLY | B | 163 | 30.805 | 12.749 | 61.427 | 1.00 | 30.91 | N |
| ATOM | 3131 | CA | GLY | B | 163 | 30.627 | 13.030 | 60.014 | 1.00 | 33.09 | C |
| ATOM | 3132 | C | GLY | B | 163 | 29.326 | 13.741 | 59.666 | 1.00 | 34.48 | C |
| ATOM | 3133 | O | GLY | B | 163 | 29.259 | 14.456 | 58.661 | 1.00 | 34.96 | O |
| ATOM | 3134 | N | LEU | B | 164 | 28.301 | 13.559 | 60.498 | 1.00 | 36.01 | N |
| ATOM | 3135 | CA | LEU | B | 164 | 26.950 | 14.040 | 60.201 | 1.00 | 37.70 | C |
| ATOM | 3136 | C | LEU | B | 164 | 26.807 | 15.557 | 60.302 | 1.00 | 39.33 | C |
| ATOM | 3137 | O | LEU | B | 164 | 25.954 | 16.152 | 59.642 | 1.00 | 39.00 | O |
| ATOM | 3138 | CB | LEU | B | 164 | 25.926 | 13.344 | 61.104 | 1.00 | 37.52 | C |
| ATOM | 3139 | CG | LEU | B | 164 | 24.988 | 12.306 | 60.470 | 1.00 | 37.49 | C |
| ATOM | 3140 | CD1 | LEU | B | 164 | 25.705 | 11.428 | 59.448 | 1.00 | 37.55 | C |
| ATOM | 3141 | CD2 | LEU | B | 164 | 24.338 | 11.452 | 61.533 | 1.00 | 36.19 | C |
| ATOM | 3142 | N | ALA | B | 165 | 27.640 | 16.172 | 61.136 | 1.00 | 41.57 | N |
| ATOM | 3143 | CA | ALA | B | 165 | 27.680 | 17.626 | 61.263 | 1.00 | 43.70 | C |
| ATOM | 3144 | C | ALA | B | 165 | 28.175 | 18.244 | 59.961 | 1.00 | 44.90 | C |
| ATOM | 3145 | O | ALA | B | 165 | 27.652 | 19.264 | 59.513 | 1.00 | 45.48 | O |
| ATOM | 3146 | CB | ALA | B | 165 | 28.576 | 18.038 | 62.431 | 1.00 | 43.57 | C |
| ATOM | 3147 | N | LYS | B | 166 | 29.178 | 17.606 | 59.360 | 1.00 | 46.41 | N |
| ATOM | 3148 | CA | LYS | B | 166 | 29.720 | 18.026 | 58.075 | 1.00 | 47.53 | C |
| ATOM | 3149 | C | LYS | B | 166 | 28.697 | 17.814 | 56.972 | 1.00 | 48.33 | C |
| ATOM | 3150 | O | LYS | B | 166 | 28.476 | 18.706 | 56.149 | 1.00 | 49.23 | O |
| ATOM | 3151 | CB | LYS | B | 166 | 30.999 | 17.248 | 57.753 | 1.00 | 47.79 | C |
| ATOM | 3152 | N | LEU | B | 167 | 28.073 | 16.635 | 56.964 | 1.00 | 48.68 | N |
| ATOM | 3153 | CA | LEU | B | 167 | 27.097 | 16.284 | 55.941 | 1.00 | 48.79 | C |
| ATOM | 3154 | C | LEU | B | 167 | 25.858 | 17.172 | 55.989 | 1.00 | 49.10 | C |
| ATOM | 3155 | O | LEU | B | 167 | 25.453 | 17.733 | 54.967 | 1.00 | 49.24 | O |
| ATOM | 3156 | CB | LEU | B | 167 | 26.701 | 14.809 | 56.056 | 1.00 | 49.03 | C |
| ATOM | 3157 | CG | LEU | B | 167 | 27.548 | 13.783 | 55.293 | 1.00 | 49.18 | C |
| ATOM | 3158 | CD1 | LEU | B | 167 | 26.913 | 12.395 | 55.361 | 1.00 | 48.70 | C |
| ATOM | 3159 | CD2 | LEU | B | 167 | 27.771 | 14.203 | 53.837 | 1.00 | 49.44 | C |
| ATOM | 3160 | N | LEU | B | 168 | 25.271 | 17.313 | 57.176 | 1.00 | 49.06 | N |
| ATOM | 3161 | CA | LEU | B | 168 | 24.001 | 18.024 | 57.324 | 1.00 | 49.05 | C |
| ATOM | 3162 | C | LEU | B | 168 | 24.163 | 19.409 | 57.948 | 1.00 | 49.23 | C |
| ATOM | 3163 | O | LEU | B | 168 | 25.140 | 20.115 | 57.683 | 1.00 | 49.32 | O |
| ATOM | 3164 | CB | LEU | B | 168 | 23.007 | 17.185 | 58.136 | 1.00 | 49.07 | C |
| ATOM | 3165 | CG | LEU | B | 168 | 22.897 | 15.681 | 57.853 | 1.00 | 48.90 | C |
| ATOM | 3166 | CD1 | LEU | B | 168 | 21.821 | 15.067 | 58.719 | 1.00 | 49.15 | C |
| ATOM | 3167 | CD2 | LEU | B | 168 | 22.615 | 15.391 | 56.383 | 1.00 | 49.34 | C |
| ATOM | 3168 | N | VAL | B | 182 | 24.642 | 25.135 | 65.216 | 1.00 | 30.57 | N |
| ATOM | 3169 | CA | VAL | B | 182 | 23.318 | 24.973 | 65.813 | 1.00 | 30.48 | C |
| ATOM | 3170 | C | VAL | B | 182 | 23.358 | 24.536 | 67.286 | 1.00 | 29.89 | C |
| ATOM | 3171 | O | VAL | B | 182 | 22.609 | 25.090 | 68.102 | 1.00 | 31.11 | O |
| ATOM | 3172 | CB | VAL | B | 182 | 22.422 | 24.007 | 65.000 | 1.00 | 30.78 | C |
| ATOM | 3173 | N | PRO | B | 183 | 24.217 | 23.572 | 67.641 | 1.00 | 28.74 | N |
| ATOM | 3174 | CA | PRO | B | 183 | 24.313 | 23.126 | 69.034 | 1.00 | 26.76 | C |

FIG. 5AAA

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3175 | C | PRO | B | 183 | 25.275 | 24.027 | 69.802 | 1.00 | 24.78 | C |
| ATOM | 3176 | O | PRO | B | 183 | 26.283 | 23.569 | 70.355 | 1.00 | 23.84 | O |
| ATOM | 3177 | CB | PRO | B | 183 | 24.866 | 21.707 | 68.905 | 1.00 | 27.33 | C |
| ATOM | 3178 | CG | PRO | B | 183 | 25.709 | 21.733 | 67.648 | 1.00 | 28.32 | C |
| ATOM | 3179 | CD | PRO | B | 183 | 25.170 | 22.844 | 66.776 | 1.00 | 28.73 | C |
| ATOM | 3180 | N | ILE | B | 184 | 24.934 | 25.313 | 69.830 | 1.00 | 22.44 | N |
| ATOM | 3181 | CA | ILE | B | 184 | 25.755 | 26.352 | 70.446 | 1.00 | 20.73 | C |
| ATOM | 3182 | C | ILE | B | 184 | 26.263 | 25.982 | 71.850 | 1.00 | 19.72 | C |
| ATOM | 3183 | O | ILE | B | 184 | 27.400 | 26.301 | 72.203 | 1.00 | 19.10 | O |
| ATOM | 3184 | CB | ILE | B | 184 | 24.975 | 27.706 | 70.465 | 1.00 | 20.48 | C |
| ATOM | 3185 | CG1 | ILE | B | 184 | 24.634 | 28.179 | 69.038 | 1.00 | 21.10 | C |
| ATOM | 3186 | CD1 | ILE | B | 184 | 25.821 | 28.262 | 68.097 | 1.00 | 21.14 | C |
| ATOM | 3187 | CG2 | ILE | B | 184 | 25.742 | 28.784 | 71.215 | 1.00 | 19.99 | C |
| ATOM | 3188 | N | LYS | B | 185 | 25.430 | 25.294 | 72.630 | 1.00 | 18.51 | N |
| ATOM | 3189 | CA | LYS | B | 185 | 25.724 | 25.044 | 74.046 | 1.00 | 17.63 | C |
| ATOM | 3190 | C | LYS | B | 185 | 26.772 | 23.959 | 74.314 | 1.00 | 17.32 | C |
| ATOM | 3191 | O | LYS | B | 185 | 27.221 | 23.790 | 75.450 | 1.00 | 17.41 | O |
| ATOM | 3192 | CB | LYS | B | 185 | 24.433 | 24.765 | 74.817 | 1.00 | 17.72 | C |
| ATOM | 3193 | CG | LYS | B | 185 | 23.580 | 26.002 | 75.013 | 1.00 | 16.63 | C |
| ATOM | 3194 | CD | LYS | B | 185 | 22.196 | 25.655 | 75.491 | 1.00 | 15.05 | C |
| ATOM | 3195 | CE | LYS | B | 185 | 21.315 | 26.885 | 75.523 | 1.00 | 13.12 | C |
| ATOM | 3196 | NZ | LYS | B | 185 | 20.340 | 26.831 | 76.661 | 1.00 | 12.44 | N |
| ATOM | 3197 | N | TRP | B | 186 | 27.170 | 23.240 | 73.265 | 1.00 | 17.19 | N |
| ATOM | 3198 | CA | TRP | B | 186 | 28.212 | 22.218 | 73.370 | 1.00 | 16.56 | C |
| ATOM | 3199 | C | TRP | B | 186 | 29.500 | 22.701 | 72.696 | 1.00 | 17.00 | C |
| ATOM | 3200 | O | TRP | B | 186 | 30.542 | 22.049 | 72.777 | 1.00 | 16.89 | O |
| ATOM | 3201 | CB | TRP | B | 186 | 27.735 | 20.894 | 72.752 | 1.00 | 15.17 | C |
| ATOM | 3202 | CG | TRP | B | 186 | 26.875 | 20.100 | 73.683 | 1.00 | 13.57 | C |
| ATOM | 3203 | CD1 | TRP | B | 186 | 27.269 | 19.055 | 74.482 | 1.00 | 12.74 | C |
| ATOM | 3204 | NE1 | TRP | B | 186 | 26.201 | 18.591 | 75.214 | 1.00 | 11.84 | N |
| ATOM | 3205 | CE2 | TRP | B | 186 | 25.091 | 19.329 | 74.898 | 1.00 | 10.92 | C |
| ATOM | 3206 | CD2 | TRP | B | 186 | 25.478 | 20.282 | 73.928 | 1.00 | 10.84 | C |
| ATOM | 3207 | CE3 | TRP | B | 186 | 24.510 | 21.171 | 73.441 | 1.00 | 11.80 | C |
| ATOM | 3208 | CZ3 | TRP | B | 186 | 23.204 | 21.082 | 73.925 | 1.00 | 11.60 | C |
| ATOM | 3209 | CH2 | TRP | B | 186 | 22.850 | 20.117 | 74.878 | 1.00 | 11.91 | C |
| ATOM | 3210 | CZ2 | TRP | B | 186 | 23.780 | 19.232 | 75.379 | 1.00 | 12.23 | C |
| ATOM | 3211 | N | MET | B | 187 | 29.417 | 23.846 | 72.027 | 1.00 | 17.15 | N |
| ATOM | 3212 | CA | MET | B | 187 | 30.534 | 24.342 | 71.222 | 1.00 | 17.93 | C |
| ATOM | 3213 | C | MET | B | 187 | 31.559 | 25.129 | 72.039 | 1.00 | 17.47 | C |
| ATOM | 3214 | O | MET | B | 187 | 31.201 | 25.940 | 72.898 | 1.00 | 17.04 | O |
| ATOM | 3215 | CB | MET | B | 187 | 30.030 | 25.195 | 70.054 | 1.00 | 18.13 | C |
| ATOM | 3216 | CG | MET | B | 187 | 29.294 | 24.410 | 68.960 | 1.00 | 20.34 | C |
| ATOM | 3217 | SD | MET | B | 187 | 28.350 | 25.493 | 67.822 | 1.00 | 23.46 | S |
| ATOM | 3218 | CE | MET | B | 187 | 29.652 | 26.213 | 66.933 | 1.00 | 22.27 | C |
| ATOM | 3219 | N | ALA | B | 188 | 32.836 | 24.862 | 71.769 | 1.00 | 17.52 | N |
| ATOM | 3220 | CA | ALA | B | 188 | 33.933 | 25.698 | 72.256 | 1.00 | 17.56 | C |
| ATOM | 3221 | C | ALA | B | 188 | 33.760 | 27.120 | 71.735 | 1.00 | 17.32 | C |
| ATOM | 3222 | O | ALA | B | 188 | 33.158 | 27.316 | 70.677 | 1.00 | 17.45 | O |
| ATOM | 3223 | CB | ALA | B | 188 | 35.246 | 25.129 | 71.796 | 1.00 | 17.47 | C |
| ATOM | 3224 | N | LEU | B | 189 | 34.266 | 28.107 | 72.474 | 1.00 | 18.04 | N |
| ATOM | 3225 | CA | LEU | B | 189 | 34.093 | 29.523 | 72.092 | 1.00 | 17.98 | C |
| ATOM | 3226 | C | LEU | B | 189 | 34.634 | 29.852 | 70.697 | 1.00 | 18.25 | C |
| ATOM | 3227 | O | LEU | B | 189 | 34.030 | 30.646 | 69.971 | 1.00 | 18.68 | O |
| ATOM | 3228 | CB | LEU | B | 189 | 34.694 | 30.484 | 73.130 | 1.00 | 17.64 | C |
| ATOM | 3229 | CG | LEU | B | 189 | 34.454 | 31.989 | 72.852 | 1.00 | 17.66 | C |
| ATOM | 3230 | CD1 | LEU | B | 189 | 32.978 | 32.404 | 72.987 | 1.00 | 14.66 | C |
| ATOM | 3231 | CD2 | LEU | B | 189 | 35.333 | 32.878 | 73.713 | 1.00 | 16.44 | C |
| ATOM | 3232 | N | GLU | B | 190 | 35.758 | 29.235 | 70.326 | 1.00 | 17.93 | N |
| ATOM | 3233 | CA | GLU | B | 190 | 36.374 | 29.452 | 69.013 | 1.00 | 17.93 | C |
| ATOM | 3234 | C | GLU | B | 190 | 35.531 | 28.862 | 67.878 | 1.00 | 18.84 | C |

FIG. 5BBB

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3235 | O | GLU | B | 190 | 35.630 | 29.291 | 66.721 | 1.00 | 18.21 | O |
| ATOM | 3236 | CB | GLU | B | 190 | 37.816 | 28.917 | 68.981 | 1.00 | 17.55 | C |
| ATOM | 3237 | CG | GLU | B | 190 | 37.946 | 27.399 | 69.036 | 1.00 | 15.77 | C |
| ATOM | 3238 | CD | GLU | B | 190 | 38.074 | 26.860 | 70.443 | 1.00 | 14.66 | C |
| ATOM | 3239 | OE1 | GLU | B | 190 | 38.558 | 25.714 | 70.591 | 1.00 | 15.90 | O |
| ATOM | 3240 | OE2 | GLU | B | 190 | 37.682 | 27.557 | 71.401 | 1.00 | 13.45 | O |
| ATOM | 3241 | N | SER | B | 191 | 34.685 | 27.892 | 68.229 | 1.00 | 19.59 | N |
| ATOM | 3242 | CA | SER | B | 191 | 33.729 | 27.315 | 67.284 | 1.00 | 20.51 | C |
| ATOM | 3243 | C | SER | B | 191 | 32.535 | 28.237 | 67.024 | 1.00 | 21.04 | C |
| ATOM | 3244 | O | SER | B | 191 | 32.108 | 28.370 | 65.877 | 1.00 | 22.17 | O |
| ATOM | 3245 | CB | SER | B | 191 | 33.251 | 25.946 | 67.769 | 1.00 | 20.44 | C |
| ATOM | 3246 | OG | SER | B | 191 | 34.347 | 25.079 | 67.989 | 1.00 | 19.95 | O |
| ATOM | 3247 | N | ILE | B | 192 | 31.996 | 28.864 | 68.073 | 1.00 | 20.89 | N |
| ATOM | 3248 | CA | ILE | B | 192 | 30.862 | 29.775 | 67.917 | 1.00 | 21.01 | C |
| ATOM | 3249 | C | ILE | B | 192 | 31.264 | 31.046 | 67.173 | 1.00 | 21.77 | C |
| ATOM | 3250 | O | ILE | B | 192 | 30.579 | 31.476 | 66.246 | 1.00 | 21.72 | O |
| ATOM | 3251 | CB | ILE | B | 192 | 30.235 | 30.178 | 69.277 | 1.00 | 20.75 | C |
| ATOM | 3252 | CG1 | ILE | B | 192 | 29.902 | 28.948 | 70.128 | 1.00 | 20.56 | C |
| ATOM | 3253 | CD1 | ILE | B | 192 | 29.511 | 29.265 | 71.554 | 1.00 | 20.43 | C |
| ATOM | 3254 | CG2 | ILE | B | 192 | 28.981 | 31.008 | 69.033 | 1.00 | 19.75 | C |
| ATOM | 3255 | N | LEU | B | 193 | 32.372 | 31.647 | 67.601 | 1.00 | 21.81 | N |
| ATOM | 3256 | CA | LEU | B | 193 | 32.801 | 32.922 | 67.062 | 1.00 | 22.13 | C |
| ATOM | 3257 | C | LEU | B | 193 | 33.411 | 32.815 | 65.660 | 1.00 | 22.73 | C |
| ATOM | 3258 | O | LEU | B | 193 | 33.131 | 33.655 | 64.804 | 1.00 | 23.38 | O |
| ATOM | 3259 | CB | LEU | B | 193 | 33.760 | 33.617 | 68.034 | 1.00 | 21.79 | C |
| ATOM | 3260 | CG | LEU | B | 193 | 33.213 | 34.093 | 69.392 | 1.00 | 20.95 | C |
| ATOM | 3261 | CD1 | LEU | B | 193 | 34.338 | 34.710 | 70.241 | 1.00 | 20.07 | C |
| ATOM | 3262 | CD2 | LEU | B | 193 | 32.051 | 35.078 | 69.236 | 1.00 | 20.51 | C |
| ATOM | 3263 | N | HIS | B | 194 | 34.212 | 31.777 | 65.415 | 1.00 | 23.10 | N |
| ATOM | 3264 | CA | HIS | B | 194 | 35.023 | 31.709 | 64.201 | 1.00 | 23.16 | C |
| ATOM | 3265 | C | HIS | B | 194 | 34.867 | 30.436 | 63.390 | 1.00 | 24.53 | C |
| ATOM | 3266 | O | HIS | B | 194 | 35.592 | 30.231 | 62.409 | 1.00 | 25.58 | O |
| ATOM | 3267 | CB | HIS | B | 194 | 36.504 | 31.882 | 64.546 | 1.00 | 22.41 | C |
| ATOM | 3268 | CG | HIS | B | 194 | 36.782 | 32.994 | 65.507 | 1.00 | 20.63 | C |
| ATOM | 3269 | ND1 | HIS | B | 194 | 37.541 | 32.818 | 66.642 | 1.00 | 20.09 | N |
| ATOM | 3270 | CE1 | HIS | B | 194 | 37.622 | 33.964 | 67.298 | 1.00 | 19.64 | C |
| ATOM | 3271 | NE2 | HIS | B | 194 | 36.947 | 34.878 | 66.622 | 1.00 | 18.91 | N |
| ATOM | 3272 | CD2 | HIS | B | 194 | 36.416 | 34.299 | 65.496 | 1.00 | 19.45 | C |
| ATOM | 3273 | N | ARG | B | 195 | 33.937 | 29.575 | 63.789 | 1.00 | 25.55 | N |
| ATOM | 3274 | CA | ARG | B | 195 | 33.792 | 28.250 | 63.171 | 1.00 | 26.11 | C |
| ATOM | 3275 | C | ARG | B | 195 | 35.124 | 27.493 | 63.036 | 1.00 | 25.03 | C |
| ATOM | 3276 | O | ARG | B | 195 | 35.371 | 26.843 | 62.024 | 1.00 | 25.43 | O |
| ATOM | 3277 | CB | ARG | B | 195 | 33.072 | 28.342 | 61.816 | 1.00 | 27.35 | C |
| ATOM | 3278 | CG | ARG | B | 195 | 31.648 | 28.872 | 61.889 | 1.00 | 30.34 | C |
| ATOM | 3279 | CD | ARG | B | 195 | 31.491 | 30.297 | 61.356 | 1.00 | 35.48 | C |
| ATOM | 3280 | NE | ARG | B | 195 | 30.871 | 31.192 | 62.342 | 1.00 | 38.85 | N |
| ATOM | 3281 | CZ | ARG | B | 195 | 29.715 | 31.832 | 62.163 | 1.00 | 40.63 | C |
| ATOM | 3282 | NH1 | ARG | B | 195 | 29.239 | 32.622 | 63.122 | 1.00 | 41.26 | N |
| ATOM | 3283 | NH2 | ARG | B | 195 | 29.036 | 31.693 | 61.029 | 1.00 | 41.16 | N |
| ATOM | 3284 | N | ILE | B | 196 | 35.973 | 27.586 | 64.061 | 1.00 | 23.94 | N |
| ATOM | 3285 | CA | ILE | B | 196 | 37.173 | 26.753 | 64.156 | 1.00 | 22.84 | C |
| ATOM | 3286 | C | ILE | B | 196 | 36.864 | 25.477 | 64.933 | 1.00 | 22.78 | C |
| ATOM | 3287 | O | ILE | B | 196 | 36.369 | 25.522 | 66.061 | 1.00 | 22.75 | O |
| ATOM | 3288 | CB | ILE | B | 196 | 38.350 | 27.499 | 64.835 | 1.00 | 22.62 | C |
| ATOM | 3289 | CG1 | ILE | B | 196 | 38.796 | 28.704 | 64.001 | 1.00 | 22.45 | C |
| ATOM | 3290 | CD1 | ILE | B | 196 | 39.518 | 29.751 | 64.809 | 1.00 | 21.32 | C |
| ATOM | 3291 | CG2 | ILE | B | 196 | 39.532 | 26.540 | 65.094 | 1.00 | 21.39 | C |
| ATOM | 3292 | N | TYR | B | 197 | 37.179 | 24.343 | 64.321 | 1.00 | 21.98 | N |
| ATOM | 3293 | CA | TYR | B | 197 | 36.925 | 23.056 | 64.925 | 1.00 | 21.05 | C |
| ATOM | 3294 | C | TYR | B | 197 | 38.201 | 22.241 | 64.951 | 1.00 | 19.95 | C |

FIG. 5CCC

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3295 | O | TYR | B | 197 | 38.829 | 22.027 | 63.913 | 1.00 | 19.38 | O |
| ATOM | 3296 | CB | TYR | B | 197 | 35.844 | 22.317 | 64.153 | 1.00 | 21.43 | C |
| ATOM | 3297 | CG | TYR | B | 197 | 34.476 | 22.939 | 64.268 | 1.00 | 23.34 | C |
| ATOM | 3298 | CD1 | TYR | B | 197 | 33.623 | 22.596 | 65.319 | 1.00 | 23.78 | C |
| ATOM | 3299 | CE1 | TYR | B | 197 | 32.352 | 23.160 | 65.429 | 1.00 | 24.21 | C |
| ATOM | 3300 | CZ | TYR | B | 197 | 31.926 | 24.064 | 64.476 | 1.00 | 25.67 | C |
| ATOM | 3301 | OH | TYR | B | 197 | 30.669 | 24.607 | 64.585 | 1.00 | 28.55 | O |
| ATOM | 3302 | CE2 | TYR | B | 197 | 32.755 | 24.432 | 63.418 | 1.00 | 24.67 | C |
| ATOM | 3303 | CD2 | TYR | B | 197 | 34.023 | 23.866 | 63.319 | 1.00 | 24.41 | C |
| ATOM | 3304 | N | THR | B | 198 | 38.586 | 21.816 | 66.152 | 1.00 | 18.61 | N |
| ATOM | 3305 | CA | THR | B | 198 | 39.786 | 21.022 | 66.348 | 1.00 | 17.89 | C |
| ATOM | 3306 | C | THR | B | 198 | 39.526 | 19.955 | 67.400 | 1.00 | 17.66 | C |
| ATOM | 3307 | O | THR | B | 198 | 38.458 | 19.904 | 68.013 | 1.00 | 17.23 | O |
| ATOM | 3308 | CB | THR | B | 198 | 40.964 | 21.889 | 66.824 | 1.00 | 17.94 | C |
| ATOM | 3309 | OG1 | THR | B | 198 | 40.676 | 22.388 | 68.138 | 1.00 | 17.72 | O |
| ATOM | 3310 | CG2 | THR | B | 198 | 41.150 | 23.156 | 65.950 | 1.00 | 17.22 | C |
| ATOM | 3311 | N | HIS | B | 199 | 40.533 | 19.121 | 67.618 | 1.00 | 16.63 | N |
| ATOM | 3312 | CA | HIS | B | 199 | 40.508 | 18.175 | 68.710 | 1.00 | 16.44 | C |
| ATOM | 3313 | C | HIS | B | 199 | 40.353 | 18.876 | 70.059 | 1.00 | 15.36 | C |
| ATOM | 3314 | O | HIS | B | 199 | 39.738 | 18.334 | 70.960 | 1.00 | 15.25 | O |
| ATOM | 3315 | CB | HIS | B | 199 | 41.753 | 17.300 | 68.653 | 1.00 | 16.22 | C |
| ATOM | 3316 | CG | HIS | B | 199 | 42.050 | 16.792 | 67.277 | 1.00 | 17.04 | C |
| ATOM | 3317 | ND1 | HIS | B | 199 | 43.203 | 17.116 | 66.593 | 1.00 | 16.89 | N |
| ATOM | 3318 | CE1 | HIS | B | 199 | 43.187 | 16.528 | 65.409 | 1.00 | 16.93 | C |
| ATOM | 3319 | NE2 | HIS | B | 199 | 42.066 | 15.837 | 65.301 | 1.00 | 17.10 | N |
| ATOM | 3320 | CD2 | HIS | B | 199 | 41.336 | 15.986 | 66.454 | 1.00 | 16.83 | C |
| ATOM | 3321 | N | GLN | B | 200 | 40.880 | 20.093 | 70.175 | 1.00 | 14.89 | N |
| ATOM | 3322 | CA | GLN | B | 200 | 40.728 | 20.887 | 71.402 | 1.00 | 14.19 | C |
| ATOM | 3323 | C | GLN | B | 200 | 39.349 | 21.529 | 71.556 | 1.00 | 13.87 | C |
| ATOM | 3324 | O | GLN | B | 200 | 38.896 | 21.756 | 72.686 | 1.00 | 13.67 | O |
| ATOM | 3325 | CB | GLN | B | 200 | 41.842 | 21.934 | 71.539 | 1.00 | 14.30 | C |
| ATOM | 3326 | CG | GLN | B | 200 | 43.222 | 21.339 | 71.765 | 1.00 | 13.95 | C |
| ATOM | 3327 | CD | GLN | B | 200 | 43.252 | 20.383 | 72.949 | 1.00 | 13.26 | C |
| ATOM | 3328 | OE1 | GLN | B | 200 | 43.076 | 19.179 | 72.787 | 1.00 | 15.04 | O |
| ATOM | 3329 | NE2 | GLN | B | 200 | 43.459 | 20.919 | 74.131 | 1.00 | 13.53 | N |
| ATOM | 3330 | N | SER | B | 201 | 38.676 | 21.812 | 70.442 | 1.00 | 13.58 | N |
| ATOM | 3331 | CA | SER | B | 201 | 37.272 | 22.233 | 70.520 | 1.00 | 13.82 | C |
| ATOM | 3332 | C | SER | B | 201 | 36.383 | 21.044 | 70.905 | 1.00 | 14.01 | C |
| ATOM | 3333 | O | SER | B | 201 | 35.402 | 21.202 | 71.631 | 1.00 | 13.85 | O |
| ATOM | 3334 | CB | SER | B | 201 | 36.794 | 22.961 | 69.247 | 1.00 | 14.05 | C |
| ATOM | 3335 | OG | SER | B | 201 | 36.793 | 22.150 | 68.086 | 1.00 | 15.63 | O |
| ATOM | 3336 | N | ASP | B | 202 | 36.757 | 19.851 | 70.441 | 1.00 | 13.39 | N |
| ATOM | 3337 | CA | ASP | B | 202 | 36.126 | 18.614 | 70.878 | 1.00 | 12.98 | C |
| ATOM | 3338 | C | ASP | B | 202 | 36.277 | 18.411 | 72.392 | 1.00 | 12.86 | C |
| ATOM | 3339 | O | ASP | B | 202 | 35.358 | 17.906 | 73.047 | 1.00 | 12.56 | O |
| ATOM | 3340 | CB | ASP | B | 202 | 36.723 | 17.416 | 70.124 | 1.00 | 13.56 | C |
| ATOM | 3341 | CG | ASP | B | 202 | 36.026 | 17.145 | 68.793 | 1.00 | 13.85 | C |
| ATOM | 3342 | OD1 | ASP | B | 202 | 36.490 | 16.243 | 68.058 | 1.00 | 13.90 | O |
| ATOM | 3343 | OD2 | ASP | B | 202 | 35.011 | 17.769 | 68.403 | 1.00 | 13.40 | O |
| ATOM | 3344 | N | VAL | B | 203 | 37.435 | 18.792 | 72.941 | 1.00 | 12.00 | N |
| ATOM | 3345 | CA | VAL | B | 203 | 37.681 | 18.658 | 74.372 | 1.00 | 12.04 | C |
| ATOM | 3346 | C | VAL | B | 203 | 36.645 | 19.473 | 75.146 | 1.00 | 11.95 | C |
| ATOM | 3347 | O | VAL | B | 203 | 36.034 | 18.975 | 76.093 | 1.00 | 12.60 | O |
| ATOM | 3348 | CB | VAL | B | 203 | 39.140 | 19.049 | 74.778 | 1.00 | 12.31 | C |
| ATOM | 3349 | CG1 | VAL | B | 203 | 39.269 | 19.222 | 76.302 | 1.00 | 11.33 | C |
| ATOM | 3350 | CG2 | VAL | B | 203 | 40.139 | 17.995 | 74.288 | 1.00 | 11.70 | C |
| ATOM | 3351 | N | TRP | B | 204 | 36.434 | 20.714 | 74.722 | 1.00 | 12.29 | N |
| ATOM | 3352 | CA | TRP | B | 204 | 35.391 | 21.553 | 75.286 | 1.00 | 12.63 | C |
| ATOM | 3353 | C | TRP | B | 204 | 34.048 | 20.807 | 75.328 | 1.00 | 13.17 | C |
| ATOM | 3354 | O | TRP | B | 204 | 33.413 | 20.732 | 76.378 | 1.00 | 13.58 | O |

FIG. 5DDD

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3355 | CB | TRP | B | 204 | 35.268 | 22.872 | 74.503 | 1.00 | 12.35 | C |
| ATOM | 3356 | CG | TRP | B | 204 | 34.253 | 23.836 | 75.100 | 1.00 | 11.68 | C |
| ATOM | 3357 | CD1 | TRP | B | 204 | 32.909 | 23.615 | 75.273 | 1.00 | 9.91 | C |
| ATOM | 3358 | NE1 | TRP | B | 204 | 32.324 | 24.711 | 75.859 | 1.00 | 10.34 | N |
| ATOM | 3359 | CE2 | TRP | B | 204 | 33.282 | 25.666 | 76.086 | 1.00 | 10.62 | C |
| ATOM | 3360 | CD2 | TRP | B | 204 | 34.510 | 25.150 | 75.618 | 1.00 | 10.49 | C |
| ATOM | 3361 | CE3 | TRP | B | 204 | 35.653 | 25.948 | 75.728 | 1.00 | 10.89 | C |
| ATOM | 3362 | CZ3 | TRP | B | 204 | 35.537 | 27.219 | 76.294 | 1.00 | 11.73 | C |
| ATOM | 3363 | CH2 | TRP | B | 204 | 34.305 | 27.704 | 76.752 | 1.00 | 10.91 | C |
| ATOM | 3364 | CZ2 | TRP | B | 204 | 33.166 | 26.949 | 76.657 | 1.00 | 11.17 | C |
| ATOM | 3365 | N | SER | B | 205 | 33.635 | 20.258 | 74.184 | 1.00 | 13.45 | N |
| ATOM | 3366 | CA | SER | B | 205 | 32.371 | 19.526 | 74.059 | 1.00 | 13.46 | C |
| ATOM | 3367 | C | SER | B | 205 | 32.309 | 18.335 | 75.009 | 1.00 | 12.99 | C |
| ATOM | 3368 | O | SER | B | 205 | 31.262 | 18.058 | 75.594 | 1.00 | 12.79 | O |
| ATOM | 3369 | CB | SER | B | 205 | 32.171 | 19.050 | 72.621 | 1.00 | 13.44 | C |
| ATOM | 3370 | OG | SER | B | 205 | 32.099 | 20.149 | 71.740 | 1.00 | 14.45 | O |
| ATOM | 3371 | N | TYR | B | 206 | 33.441 | 17.639 | 75.142 | 1.00 | 13.17 | N |
| ATOM | 3372 | CA | TYR | B | 206 | 33.609 | 16.547 | 76.106 | 1.00 | 12.53 | C |
| ATOM | 3373 | C | TYR | B | 206 | 33.365 | 17.014 | 77.543 | 1.00 | 11.99 | C |
| ATOM | 3374 | O | TYR | B | 206 | 32.758 | 16.305 | 78.323 | 1.00 | 12.39 | O |
| ATOM | 3375 | CB | TYR | B | 206 | 35.008 | 15.923 | 75.970 | 1.00 | 12.35 | C |
| ATOM | 3376 | CG | TYR | B | 206 | 35.313 | 14.851 | 76.994 | 1.00 | 12.39 | C |
| ATOM | 3377 | CD1 | TYR | B | 206 | 35.838 | 15.183 | 78.249 | 1.00 | 12.59 | C |
| ATOM | 3378 | CE1 | TYR | B | 206 | 36.121 | 14.190 | 79.207 | 1.00 | 12.82 | C |
| ATOM | 3379 | CZ | TYR | B | 206 | 35.874 | 12.860 | 78.907 | 1.00 | 12.21 | C |
| ATOM | 3380 | OH | TYR | B | 206 | 36.142 | 11.892 | 79.853 | 1.00 | 13.41 | O |
| ATOM | 3381 | CE2 | TYR | B | 206 | 35.348 | 12.504 | 77.670 | 1.00 | 11.74 | C |
| ATOM | 3382 | CD2 | TYR | B | 206 | 35.064 | 13.500 | 76.719 | 1.00 | 11.49 | C |
| ATOM | 3383 | N | GLY | B | 207 | 33.834 | 18.207 | 77.892 | 1.00 | 11.78 | N |
| ATOM | 3384 | CA | GLY | B | 207 | 33.565 | 18.765 | 79.206 | 1.00 | 11.79 | C |
| ATOM | 3385 | C | GLY | B | 207 | 32.068 | 18.917 | 79.493 | 1.00 | 12.46 | C |
| ATOM | 3386 | O | GLY | B | 207 | 31.610 | 18.609 | 80.605 | 1.00 | 11.86 | O |
| ATOM | 3387 | N | VAL | B | 208 | 31.322 | 19.408 | 78.495 | 1.00 | 11.34 | N |
| ATOM | 3388 | CA | VAL | B | 208 | 29.875 | 19.594 | 78.601 | 1.00 | 11.23 | C |
| ATOM | 3389 | C | VAL | B | 208 | 29.146 | 18.242 | 78.673 | 1.00 | 11.48 | C |
| ATOM | 3390 | O | VAL | B | 208 | 28.161 | 18.093 | 79.396 | 1.00 | 10.39 | O |
| ATOM | 3391 | CB | VAL | B | 208 | 29.298 | 20.441 | 77.407 | 1.00 | 11.76 | C |
| ATOM | 3392 | CG1 | VAL | B | 208 | 27.803 | 20.687 | 77.580 | 1.00 | 11.13 | C |
| ATOM | 3393 | CG2 | VAL | B | 208 | 30.025 | 21.777 | 77.258 | 1.00 | 10.06 | C |
| ATOM | 3394 | N | THR | B | 209 | 29.656 | 17.263 | 77.926 | 1.00 | 11.61 | N |
| ATOM | 3395 | CA | THR | B | 209 | 29.079 | 15.935 | 77.873 | 1.00 | 11.60 | C |
| ATOM | 3396 | C | THR | B | 209 | 29.180 | 15.226 | 79.215 | 1.00 | 11.88 | C |
| ATOM | 3397 | O | THR | B | 209 | 28.214 | 14.596 | 79.657 | 1.00 | 11.75 | O |
| ATOM | 3398 | CB | THR | B | 209 | 29.749 | 15.144 | 76.743 | 1.00 | 12.45 | C |
| ATOM | 3399 | OG1 | THR | B | 209 | 29.447 | 15.790 | 75.494 | 1.00 | 13.45 | O |
| ATOM | 3400 | CG2 | THR | B | 209 | 29.150 | 13.744 | 76.594 | 1.00 | 10.29 | C |
| ATOM | 3401 | N | VAL | B | 210 | 30.339 | 15.358 | 79.865 | 1.00 | 12.22 | N |
| ATOM | 3402 | CA | VAL | B | 210 | 30.558 | 14.854 | 81.226 | 1.00 | 11.90 | C |
| ATOM | 3403 | C | VAL | B | 210 | 29.629 | 15.559 | 82.227 | 1.00 | 11.86 | C |
| ATOM | 3404 | O | VAL | B | 210 | 29.067 | 14.909 | 83.128 | 1.00 | 12.05 | O |
| ATOM | 3405 | CB | VAL | B | 210 | 32.049 | 14.982 | 81.637 | 1.00 | 12.02 | C |
| ATOM | 3406 | CG1 | VAL | B | 210 | 32.243 | 14.780 | 83.138 | 1.00 | 12.94 | C |
| ATOM | 3407 | CG2 | VAL | B | 210 | 32.886 | 13.986 | 80.871 | 1.00 | 12.66 | C |
| ATOM | 3408 | N | TRP | B | 211 | 29.449 | 16.872 | 82.060 | 1.00 | 11.36 | N |
| ATOM | 3409 | CA | TRP | B | 211 | 28.499 | 17.634 | 82.886 | 1.00 | 11.24 | C |
| ATOM | 3410 | C | TRP | B | 211 | 27.089 | 17.046 | 82.762 | 1.00 | 11.43 | C |
| ATOM | 3411 | O | TRP | B | 211 | 26.408 | 16.841 | 83.760 | 1.00 | 11.61 | O |
| ATOM | 3412 | CB | TRP | B | 211 | 28.508 | 19.119 | 82.521 | 1.00 | 10.51 | C |
| ATOM | 3413 | CG | TRP | B | 211 | 27.663 | 20.014 | 83.435 | 1.00 | 9.90 | C |
| ATOM | 3414 | CD1 | TRP | B | 211 | 28.079 | 20.670 | 84.565 | 1.00 | 10.06 | C |

FIG. 5EEE

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3415 | NE1 | TRP | B | 211 | 27.044 | 21.395 | 85.108 | 1.00 | 8.54 | N |
| ATOM | 3416 | CE2 | TRP | B | 211 | 25.927 | 21.225 | 84.332 | 1.00 | 9.96 | C |
| ATOM | 3417 | CD2 | TRP | B | 211 | 26.282 | 20.362 | 83.263 | 1.00 | 9.15 | C |
| ATOM | 3418 | CE3 | TRP | B | 211 | 25.299 | 20.034 | 82.309 | 1.00 | 9.01 | C |
| ATOM | 3419 | CZ3 | TRP | B | 211 | 24.008 | 20.563 | 82.457 | 1.00 | 8.15 | C |
| ATOM | 3420 | CH2 | TRP | B | 211 | 23.690 | 21.412 | 83.538 | 1.00 | 9.22 | C |
| ATOM | 3421 | CZ2 | TRP | B | 211 | 24.629 | 21.757 | 84.480 | 1.00 | 9.17 | C |
| ATOM | 3422 | N | GLU | B | 212 | 26.673 | 16.766 | 81.530 | 1.00 | 11.86 | N |
| ATOM | 3423 | CA | GLU | B | 212 | 25.389 | 16.124 | 81.249 | 1.00 | 12.21 | C |
| ATOM | 3424 | C | GLU | B | 212 | 25.227 | 14.816 | 82.015 | 1.00 | 12.72 | C |
| ATOM | 3425 | O | GLU | B | 212 | 24.205 | 14.598 | 82.666 | 1.00 | 13.19 | O |
| ATOM | 3426 | CB | GLU | B | 212 | 25.257 | 15.836 | 79.763 | 1.00 | 11.92 | C |
| ATOM | 3427 | CG | GLU | B | 212 | 24.918 | 17.027 | 78.901 | 1.00 | 13.09 | C |
| ATOM | 3428 | CD | GLU | B | 212 | 24.741 | 16.610 | 77.460 | 1.00 | 15.06 | C |
| ATOM | 3429 | OE1 | GLU | B | 212 | 25.757 | 16.505 | 76.735 | 1.00 | 12.28 | O |
| ATOM | 3430 | OE2 | GLU | B | 212 | 23.575 | 16.358 | 77.068 | 1.00 | 18.01 | O |
| ATOM | 3431 | N | LEU | B | 213 | 26.236 | 13.947 | 81.929 | 1.00 | 13.18 | N |
| ATOM | 3432 | CA | LEU | B | 213 | 26.201 | 12.654 | 82.611 | 1.00 | 13.20 | C |
| ATOM | 3433 | C | LEU | B | 213 | 26.074 | 12.800 | 84.130 | 1.00 | 13.33 | C |
| ATOM | 3434 | O | LEU | B | 213 | 25.288 | 12.104 | 84.763 | 1.00 | 13.44 | O |
| ATOM | 3435 | CB | LEU | B | 213 | 27.441 | 11.832 | 82.252 | 1.00 | 12.47 | C |
| ATOM | 3436 | CG | LEU | B | 213 | 27.604 | 11.439 | 80.777 | 1.00 | 12.45 | C |
| ATOM | 3437 | CD1 | LEU | B | 213 | 28.748 | 10.433 | 80.612 | 1.00 | 10.90 | C |
| ATOM | 3438 | CD2 | LEU | B | 213 | 26.289 | 10.889 | 80.200 | 1.00 | 11.77 | C |
| ATOM | 3439 | N | MET | B | 214 | 26.838 | 13.730 | 84.694 | 1.00 | 14.15 | N |
| ATOM | 3440 | CA | MET | B | 214 | 26.938 | 13.906 | 86.147 | 1.00 | 14.30 | C |
| ATOM | 3441 | C | MET | B | 214 | 25.723 | 14.602 | 86.754 | 1.00 | 13.92 | C |
| ATOM | 3442 | O | MET | B | 214 | 25.510 | 14.549 | 87.974 | 1.00 | 13.65 | O |
| ATOM | 3443 | CB | MET | B | 214 | 28.215 | 14.667 | 86.502 | 1.00 | 14.74 | C |
| ATOM | 3444 | CG | MET | B | 214 | 29.498 | 13.981 | 86.060 | 1.00 | 16.61 | C |
| ATOM | 3445 | SD | MET | B | 214 | 29.819 | 12.457 | 86.939 | 1.00 | 20.02 | S |
| ATOM | 3446 | CE | MET | B | 214 | 31.210 | 11.834 | 86.063 | 1.00 | 19.98 | C |
| ATOM | 3447 | N | THR | B | 215 | 24.934 | 15.256 | 85.904 | 1.00 | 13.54 | N |
| ATOM | 3448 | CA | THR | B | 215 | 23.656 | 15.826 | 86.322 | 1.00 | 13.05 | C |
| ATOM | 3449 | C | THR | B | 215 | 22.499 | 14.943 | 85.863 | 1.00 | 13.03 | C |
| ATOM | 3450 | O | THR | B | 215 | 21.344 | 15.361 | 85.896 | 1.00 | 13.13 | O |
| ATOM | 3451 | CB | THR | B | 215 | 23.486 | 17.226 | 85.723 | 1.00 | 13.30 | C |
| ATOM | 3452 | OG1 | THR | B | 215 | 23.639 | 17.149 | 84.297 | 1.00 | 13.00 | O |
| ATOM | 3453 | CG2 | THR | B | 215 | 24.608 | 18.166 | 86.189 | 1.00 | 12.58 | C |
| ATOM | 3454 | N | PHE | B | 216 | 22.817 | 13.743 | 85.383 | 1.00 | 12.98 | N |
| ATOM | 3455 | CA | PHE | B | 216 | 21.812 | 12.787 | 84.909 | 1.00 | 12.93 | C |
| ATOM | 3456 | C | PHE | B | 216 | 20.943 | 13.323 | 83.766 | 1.00 | 13.03 | C |
| ATOM | 3457 | O | PHE | B | 216 | 19.750 | 13.048 | 83.697 | 1.00 | 13.96 | O |
| ATOM | 3458 | CB | PHE | B | 216 | 20.957 | 12.257 | 86.080 | 1.00 | 12.68 | C |
| ATOM | 3459 | CG | PHE | B | 216 | 21.768 | 11.566 | 87.153 | 1.00 | 12.58 | C |
| ATOM | 3460 | CD1 | PHE | B | 216 | 22.230 | 10.271 | 86.960 | 1.00 | 11.60 | C |
| ATOM | 3461 | CE1 | PHE | B | 216 | 22.987 | 9.624 | 87.935 | 1.00 | 12.74 | C |
| ATOM | 3462 | CZ | PHE | B | 216 | 23.310 | 10.284 | 89.119 | 1.00 | 12.78 | C |
| ATOM | 3463 | CE2 | PHE | B | 216 | 22.858 | 11.590 | 89.323 | 1.00 | 13.24 | C |
| ATOM | 3464 | CD2 | PHE | B | 216 | 22.088 | 12.223 | 88.338 | 1.00 | 12.07 | C |
| ATOM | 3465 | N | GLY | B | 217 | 21.562 | 14.071 | 82.864 | 1.00 | 12.87 | N |
| ATOM | 3466 | CA | GLY | B | 217 | 20.902 | 14.535 | 81.660 | 1.00 | 13.32 | C |
| ATOM | 3467 | C | GLY | B | 217 | 20.224 | 15.886 | 81.780 | 1.00 | 13.37 | C |
| ATOM | 3468 | O | GLY | B | 217 | 19.185 | 16.105 | 81.163 | 1.00 | 12.73 | O |
| ATOM | 3469 | N | SER | B | 218 | 20.813 | 16.791 | 82.562 | 1.00 | 13.16 | N |
| ATOM | 3470 | CA | SER | B | 218 | 20.261 | 18.130 | 82.716 | 1.00 | 13.17 | C |
| ATOM | 3471 | C | SER | B | 218 | 20.633 | 19.024 | 81.525 | 1.00 | 13.52 | C |
| ATOM | 3472 | O | SER | B | 218 | 21.615 | 18.768 | 80.813 | 1.00 | 12.88 | O |
| ATOM | 3473 | CB | SER | B | 218 | 20.720 | 18.755 | 84.034 | 1.00 | 13.01 | C |
| ATOM | 3474 | OG | SER | B | 218 | 20.259 | 17.988 | 85.139 | 1.00 | 14.30 | O |

FIG. 5FF

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3475 | N | LYS | B | 219 | 19.837 | 20.070 | 81.315 | 1.00 | 13.68 | N |
| ATOM | 3476 | CA | LYS | B | 219 | 20.081 | 21.018 | 80.236 | 1.00 | 13.58 | C |
| ATOM | 3477 | C | LYS | B | 219 | 21.188 | 22.008 | 80.619 | 1.00 | 13.36 | C |
| ATOM | 3478 | O | LYS | B | 219 | 21.112 | 22.664 | 81.673 | 1.00 | 13.45 | O |
| ATOM | 3479 | CB | LYS | B | 219 | 18.787 | 21.746 | 79.870 | 1.00 | 13.66 | C |
| ATOM | 3480 | CG | LYS | B | 219 | 17.761 | 20.866 | 79.175 | 1.00 | 15.43 | C |
| ATOM | 3481 | CD | LYS | B | 219 | 16.324 | 21.244 | 79.537 | 1.00 | 16.23 | C |
| ATOM | 3482 | N | PRO | B | 220 | 22.228 | 22.097 | 79.785 | 1.00 | 13.07 | N |
| ATOM | 3483 | CA | PRO | B | 220 | 23.303 | 23.075 | 79.997 | 1.00 | 12.97 | C |
| ATOM | 3484 | C | PRO | B | 220 | 22.840 | 24.495 | 79.709 | 1.00 | 13.50 | C |
| ATOM | 3485 | O | PRO | B | 220 | 22.134 | 24.725 | 78.723 | 1.00 | 13.45 | O |
| ATOM | 3486 | CB | PRO | B | 220 | 24.390 | 22.648 | 78.999 | 1.00 | 12.67 | C |
| ATOM | 3487 | CG | PRO | B | 220 | 23.711 | 21.814 | 77.992 | 1.00 | 12.80 | C |
| ATOM | 3488 | CD | PRO | B | 220 | 22.465 | 21.256 | 78.599 | 1.00 | 12.47 | C |
| ATOM | 3489 | N | TYR | B | 221 | 23.237 | 25.434 | 80.571 | 1.00 | 13.83 | N |
| ATOM | 3490 | CA | TYR | B | 221 | 22.876 | 26.838 | 80.422 | 1.00 | 14.51 | C |
| ATOM | 3491 | C | TYR | B | 221 | 21.378 | 26.971 | 80.303 | 1.00 | 14.56 | C |
| ATOM | 3492 | O | TYR | B | 221 | 20.872 | 27.621 | 79.405 | 1.00 | 15.20 | O |
| ATOM | 3493 | CB | TYR | B | 221 | 23.562 | 27.469 | 79.202 | 1.00 | 14.32 | C |
| ATOM | 3494 | CG | TYR | B | 221 | 25.038 | 27.200 | 79.119 | 1.00 | 13.60 | C |
| ATOM | 3495 | CD1 | TYR | B | 221 | 25.927 | 27.812 | 79.997 | 1.00 | 13.71 | C |
| ATOM | 3496 | CE1 | TYR | B | 221 | 27.279 | 27.568 | 79.923 | 1.00 | 14.78 | C |
| ATOM | 3497 | CZ | TYR | B | 221 | 27.759 | 26.703 | 78.956 | 1.00 | 15.26 | C |
| ATOM | 3498 | OH | TYR | B | 221 | 29.106 | 26.462 | 78.868 | 1.00 | 17.47 | O |
| ATOM | 3499 | CE2 | TYR | B | 221 | 26.897 | 26.086 | 78.072 | 1.00 | 14.24 | C |
| ATOM | 3500 | CD2 | TYR | B | 221 | 25.547 | 26.339 | 78.158 | 1.00 | 14.07 | C |
| ATOM | 3501 | N | ASP | B | 222 | 20.681 | 26.315 | 81.216 | 1.00 | 16.09 | N |
| ATOM | 3502 | CA | ASP | B | 222 | 19.235 | 26.351 | 81.292 | 1.00 | 16.84 | C |
| ATOM | 3503 | C | ASP | B | 222 | 18.831 | 27.783 | 81.600 | 1.00 | 17.60 | C |
| ATOM | 3504 | O | ASP | B | 222 | 19.357 | 28.395 | 82.536 | 1.00 | 18.21 | O |
| ATOM | 3505 | CB | ASP | B | 222 | 18.780 | 25.401 | 82.403 | 1.00 | 16.45 | C |
| ATOM | 3506 | CG | ASP | B | 222 | 17.320 | 25.049 | 82.322 | 1.00 | 15.83 | C |
| ATOM | 3507 | OD1 | ASP | B | 222 | 16.699 | 25.175 | 81.231 | 1.00 | 15.41 | O |
| ATOM | 3508 | OD2 | ASP | B | 222 | 16.712 | 24.611 | 83.320 | 1.00 | 15.50 | O |
| ATOM | 3509 | N | GLY | B | 223 | 17.937 | 28.332 | 80.789 | 1.00 | 18.15 | N |
| ATOM | 3510 | CA | GLY | B | 223 | 17.547 | 29.728 | 80.934 | 1.00 | 19.05 | C |
| ATOM | 3511 | C | GLY | B | 223 | 18.352 | 30.732 | 80.124 | 1.00 | 19.50 | C |
| ATOM | 3512 | O | GLY | B | 223 | 18.049 | 31.919 | 80.176 | 1.00 | 20.10 | O |
| ATOM | 3513 | N | ILE | B | 224 | 19.382 | 30.282 | 79.396 | 1.00 | 20.10 | N |
| ATOM | 3514 | CA | ILE | B | 224 | 20.124 | 31.173 | 78.485 | 1.00 | 20.19 | C |
| ATOM | 3515 | C | ILE | B | 224 | 19.838 | 30.781 | 77.039 | 1.00 | 20.41 | C |
| ATOM | 3516 | O | ILE | B | 224 | 20.013 | 29.620 | 76.674 | 1.00 | 20.75 | O |
| ATOM | 3517 | CB | ILE | B | 224 | 21.664 | 31.168 | 78.759 | 1.00 | 20.38 | C |
| ATOM | 3518 | CG1 | ILE | B | 224 | 21.973 | 31.455 | 80.235 | 1.00 | 19.85 | C |
| ATOM | 3519 | CD1 | ILE | B | 224 | 23.430 | 31.233 | 80.599 | 1.00 | 18.90 | C |
| ATOM | 3520 | CG2 | ILE | B | 224 | 22.400 | 32.192 | 77.864 | 1.00 | 19.94 | C |
| ATOM | 3521 | N | PRO | B | 225 | 19.385 | 31.735 | 76.224 | 1.00 | 20.41 | N |
| ATOM | 3522 | CA | PRO | B | 225 | 19.148 | 31.475 | 74.796 | 1.00 | 20.58 | C |
| ATOM | 3523 | C | PRO | B | 225 | 20.475 | 31.278 | 74.060 | 1.00 | 20.74 | C |
| ATOM | 3524 | O | PRO | B | 225 | 21.480 | 31.906 | 74.416 | 1.00 | 20.85 | O |
| ATOM | 3525 | CB | PRO | B | 225 | 18.438 | 32.745 | 74.307 | 1.00 | 20.68 | C |
| ATOM | 3526 | CG | PRO | B | 225 | 18.062 | 33.522 | 75.562 | 1.00 | 20.97 | C |
| ATOM | 3527 | CD | PRO | B | 225 | 19.078 | 33.129 | 76.596 | 1.00 | 20.54 | C |
| ATOM | 3528 | N | ALA | B | 226 | 20.471 | 30.406 | 73.057 | 1.00 | 21.00 | N |
| ATOM | 3529 | CA | ALA | B | 226 | 21.679 | 30.026 | 72.319 | 1.00 | 22.30 | C |
| ATOM | 3530 | C | ALA | B | 226 | 22.485 | 31.217 | 71.793 | 1.00 | 23.01 | C |
| ATOM | 3531 | O | ALA | B | 226 | 23.716 | 31.171 | 71.771 | 1.00 | 23.39 | O |
| ATOM | 3532 | CB | ALA | B | 226 | 21.330 | 29.048 | 71.169 | 1.00 | 21.73 | C |
| ATOM | 3533 | N | SER | B | 227 | 21.787 | 32.279 | 71.382 | 1.00 | 23.77 | N |
| ATOM | 3534 | CA | SER | B | 227 | 22.430 | 33.487 | 70.848 | 1.00 | 23.79 | C |

FIG. 5GGG

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3535 | C | SER | B | 227 | 23.269 | 34.259 | 71.863 | 1.00 | 23.26 | C |
| ATOM | 3536 | O | SER | B | 227 | 24.071 | 35.103 | 71.478 | 1.00 | 23.63 | O |
| ATOM | 3537 | CB | SER | B | 227 | 21.386 | 34.430 | 70.242 | 1.00 | 24.24 | C |
| ATOM | 3538 | OG | SER | B | 227 | 20.457 | 34.855 | 71.232 | 1.00 | 25.39 | O |
| ATOM | 3539 | N | GLU | B | 228 | 23.093 | 33.968 | 73.148 | 1.00 | 22.99 | N |
| ATOM | 3540 | CA | GLU | B | 228 | 23.759 | 34.725 | 74.210 | 1.00 | 22.66 | C |
| ATOM | 3541 | C | GLU | B | 228 | 24.938 | 33.978 | 74.820 | 1.00 | 22.10 | C |
| ATOM | 3542 | O | GLU | B | 228 | 25.642 | 34.508 | 75.683 | 1.00 | 22.07 | O |
| ATOM | 3543 | CB | GLU | B | 228 | 22.762 | 35.078 | 75.311 | 1.00 | 23.05 | C |
| ATOM | 3544 | CG | GLU | B | 228 | 21.780 | 36.167 | 74.920 | 1.00 | 25.79 | C |
| ATOM | 3545 | CD | GLU | B | 228 | 22.327 | 37.559 | 75.178 | 1.00 | 27.85 | C |
| ATOM | 3546 | OE1 | GLU | B | 228 | 22.176 | 38.061 | 76.317 | 1.00 | 30.54 | O |
| ATOM | 3547 | OE2 | GLU | B | 228 | 22.910 | 38.143 | 74.248 | 1.00 | 26.71 | O |
| ATOM | 3548 | N | ILE | B | 229 | 25.151 | 32.750 | 74.364 | 1.00 | 21.35 | N |
| ATOM | 3549 | CA | ILE | B | 229 | 26.117 | 31.865 | 74.987 | 1.00 | 21.14 | C |
| ATOM | 3550 | C | ILE | B | 229 | 27.549 | 32.387 | 74.877 | 1.00 | 21.31 | C |
| ATOM | 3551 | O | ILE | B | 229 | 28.254 | 32.449 | 75.884 | 1.00 | 21.30 | O |
| ATOM | 3552 | CB | ILE | B | 229 | 25.972 | 30.415 | 74.452 | 1.00 | 20.56 | C |
| ATOM | 3553 | CG1 | ILE | B | 229 | 24.714 | 29.751 | 75.034 | 1.00 | 20.34 | C |
| ATOM | 3554 | CD1 | ILE | B | 229 | 24.642 | 29.724 | 76.558 | 1.00 | 19.28 | C |
| ATOM | 3555 | CG2 | ILE | B | 229 | 27.214 | 29.583 | 74.767 | 1.00 | 20.51 | C |
| ATOM | 3556 | N | SER | B | 230 | 27.968 | 32.774 | 73.672 | 1.00 | 21.47 | N |
| ATOM | 3557 | CA | SER | B | 230 | 29.325 | 33.285 | 73.469 | 1.00 | 22.24 | C |
| ATOM | 3558 | C | SER | B | 230 | 29.593 | 34.505 | 74.357 | 1.00 | 22.55 | C |
| ATOM | 3559 | O | SER | B | 230 | 30.708 | 34.698 | 74.849 | 1.00 | 23.52 | O |
| ATOM | 3560 | CB | SER | B | 230 | 29.608 | 33.565 | 71.982 | 1.00 | 22.20 | C |
| ATOM | 3561 | OG | SER | B | 230 | 28.830 | 34.633 | 71.465 | 1.00 | 24.03 | O |
| ATOM | 3562 | N | SER | B | 231 | 28.547 | 35.291 | 74.596 | 1.00 | 22.59 | N |
| ATOM | 3563 | CA | SER | B | 231 | 28.614 | 36.461 | 75.466 | 1.00 | 23.00 | C |
| ATOM | 3564 | C | SER | B | 231 | 28.862 | 36.106 | 76.938 | 1.00 | 22.72 | C |
| ATOM | 3565 | O | SER | B | 231 | 29.770 | 36.665 | 77.573 | 1.00 | 23.09 | O |
| ATOM | 3566 | CB | SER | B | 231 | 27.333 | 37.281 | 75.326 | 1.00 | 23.12 | C |
| ATOM | 3567 | OG | SER | B | 231 | 27.439 | 38.487 | 76.043 | 1.00 | 25.45 | O |
| ATOM | 3568 | N | ILE | B | 232 | 28.067 | 35.176 | 77.477 | 1.00 | 22.05 | N |
| ATOM | 3569 | CA | ILE | B | 232 | 28.240 | 34.741 | 78.866 | 1.00 | 21.30 | C |
| ATOM | 3570 | C | ILE | B | 232 | 29.578 | 34.012 | 79.079 | 1.00 | 21.03 | C |
| ATOM | 3571 | O | ILE | B | 232 | 30.209 | 34.166 | 80.118 | 1.00 | 20.96 | O |
| ATOM | 3572 | CB | ILE | B | 232 | 27.008 | 33.920 | 79.391 | 1.00 | 21.78 | C |
| ATOM | 3573 | CG1 | ILE | B | 232 | 26.869 | 32.554 | 78.697 | 1.00 | 21.34 | C |
| ATOM | 3574 | CD1 | ILE | B | 232 | 27.378 | 31.395 | 79.518 | 1.00 | 20.20 | C |
| ATOM | 3575 | CG2 | ILE | B | 232 | 25.705 | 34.724 | 79.235 | 1.00 | 21.34 | C |
| ATOM | 3576 | N | LEU | B | 233 | 30.025 | 33.255 | 78.081 | 1.00 | 20.86 | N |
| ATOM | 3577 | CA | LEU | B | 233 | 31.322 | 32.575 | 78.164 | 1.00 | 21.43 | C |
| ATOM | 3578 | C | LEU | B | 233 | 32.481 | 33.562 | 78.256 | 1.00 | 21.77 | C |
| ATOM | 3579 | O | LEU | B | 233 | 33.367 | 33.414 | 79.105 | 1.00 | 21.48 | O |
| ATOM | 3580 | CB | LEU | B | 233 | 31.529 | 31.620 | 76.987 | 1.00 | 20.79 | C |
| ATOM | 3581 | CG | LEU | B | 233 | 30.607 | 30.402 | 76.908 | 1.00 | 20.04 | C |
| ATOM | 3582 | CD1 | LEU | B | 233 | 30.807 | 29.705 | 75.583 | 1.00 | 19.71 | C |
| ATOM | 3583 | CD2 | LEU | B | 233 | 30.821 | 29.433 | 78.089 | 1.00 | 19.12 | C |
| ATOM | 3584 | N | GLU | B | 234 | 32.453 | 34.576 | 77.392 | 1.00 | 23.05 | N |
| ATOM | 3585 | CA | GLU | B | 234 | 33.456 | 35.648 | 77.400 | 1.00 | 24.05 | C |
| ATOM | 3586 | C | GLU | B | 234 | 33.537 | 36.370 | 78.741 | 1.00 | 23.77 | C |
| ATOM | 3587 | O | GLU | B | 234 | 34.603 | 36.845 | 79.118 | 1.00 | 23.80 | O |
| ATOM | 3588 | CB | GLU | B | 234 | 33.202 | 36.646 | 76.263 | 1.00 | 24.51 | C |
| ATOM | 3589 | CG | GLU | B | 234 | 33.719 | 36.154 | 74.922 | 1.00 | 26.00 | C |
| ATOM | 3590 | CD | GLU | B | 234 | 33.368 | 37.074 | 73.762 | 1.00 | 28.75 | C |
| ATOM | 3591 | OE1 | GLU | B | 234 | 34.277 | 37.397 | 72.973 | 1.00 | 30.25 | O |
| ATOM | 3592 | OE2 | GLU | B | 234 | 32.191 | 37.476 | 73.627 | 1.00 | 30.99 | O |
| ATOM | 3593 | N | LYS | B | 235 | 32.413 | 36.424 | 79.457 | 1.00 | 24.49 | N |
| ATOM | 3594 | CA | LYS | B | 235 | 32.340 | 37.005 | 80.797 | 1.00 | 24.93 | C |

FIG. 5HHH

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3595 | C | LYS | B | 235 | 32.902 | 36.086 | 81.877 | 1.00 | 24.45 | C |
| ATOM | 3596 | O | LYS | B | 235 | 33.078 | 36.505 | 83.024 | 1.00 | 24.35 | O |
| ATOM | 3597 | CB | LYS | B | 235 | 30.893 | 37.355 | 81.150 | 1.00 | 25.98 | C |
| ATOM | 3598 | CG | LYS | B | 235 | 30.368 | 38.618 | 80.492 | 1.00 | 28.19 | C |
| ATOM | 3599 | CD | LYS | B | 235 | 28.862 | 38.763 | 80.711 | 1.00 | 31.13 | C |
| ATOM | 3600 | CE | LYS | B | 235 | 28.557 | 39.471 | 82.032 | 1.00 | 33.15 | C |
| ATOM | 3601 | NZ | LYS | B | 235 | 27.086 | 39.595 | 82.276 | 1.00 | 35.13 | N |
| ATOM | 3602 | N | GLY | B | 236 | 33.174 | 34.836 | 81.512 | 1.00 | 24.09 | N |
| ATOM | 3603 | CA | GLY | B | 236 | 33.720 | 33.854 | 82.438 | 1.00 | 23.13 | C |
| ATOM | 3604 | C | GLY | B | 236 | 32.683 | 32.941 | 83.070 | 1.00 | 22.39 | C |
| ATOM | 3605 | O | GLY | B | 236 | 32.984 | 32.221 | 84.017 | 1.00 | 22.47 | O |
| ATOM | 3606 | N | GLU | B | 237 | 31.458 | 32.969 | 82.555 | 1.00 | 21.87 | N |
| ATOM | 3607 | CA | GLU | B | 237 | 30.410 | 32.082 | 83.055 | 1.00 | 21.59 | C |
| ATOM | 3608 | C | GLU | B | 237 | 30.594 | 30.660 | 82.537 | 1.00 | 20.08 | C |
| ATOM | 3609 | O | GLU | B | 237 | 30.942 | 30.449 | 81.372 | 1.00 | 19.72 | O |
| ATOM | 3610 | CB | GLU | B | 237 | 29.026 | 32.599 | 82.682 | 1.00 | 22.13 | C |
| ATOM | 3611 | CG | GLU | B | 237 | 28.732 | 33.985 | 83.229 | 1.00 | 26.28 | C |
| ATOM | 3612 | CD | GLU | B | 237 | 28.064 | 33.947 | 84.590 | 1.00 | 29.38 | C |
| ATOM | 3613 | OE1 | GLU | B | 237 | 28.199 | 32.928 | 85.306 | 1.00 | 31.52 | O |
| ATOM | 3614 | OE2 | GLU | B | 237 | 27.396 | 34.941 | 84.942 | 1.00 | 31.26 | O |
| ATOM | 3615 | N | ARG | B | 238 | 30.339 | 29.705 | 83.425 | 1.00 | 18.37 | N |
| ATOM | 3616 | CA | ARG | B | 238 | 30.519 | 28.289 | 83.166 | 1.00 | 17.29 | C |
| ATOM | 3617 | C | ARG | B | 238 | 29.401 | 27.486 | 83.817 | 1.00 | 16.49 | C |
| ATOM | 3618 | O | ARG | B | 238 | 28.752 | 27.943 | 84.761 | 1.00 | 17.26 | O |
| ATOM | 3619 | CB | ARG | B | 238 | 31.879 | 27.807 | 83.700 | 1.00 | 17.10 | C |
| ATOM | 3620 | CG | ARG | B | 238 | 33.110 | 28.341 | 82.955 | 1.00 | 16.95 | C |
| ATOM | 3621 | CD | ARG | B | 238 | 33.069 | 28.139 | 81.423 | 1.00 | 17.64 | C |
| ATOM | 3622 | NE | ARG | B | 238 | 34.316 | 28.581 | 80.801 | 1.00 | 17.77 | N |
| ATOM | 3623 | CZ | ARG | B | 238 | 34.563 | 29.812 | 80.386 | 1.00 | 16.60 | C |
| ATOM | 3624 | NH1 | ARG | B | 238 | 33.649 | 30.770 | 80.503 | 1.00 | 16.67 | N |
| ATOM | 3625 | NH2 | ARG | B | 238 | 35.738 | 30.085 | 79.847 | 1.00 | 17.35 | N |
| ATOM | 3626 | N | LEU | B | 239 | 29.186 | 26.283 | 83.303 | 1.00 | 15.01 | N |
| ATOM | 3627 | CA | LEU | B | 239 | 28.277 | 25.312 | 83.902 | 1.00 | 13.63 | C |
| ATOM | 3628 | C | LEU | B | 239 | 28.645 | 25.037 | 85.362 | 1.00 | 12.77 | C |
| ATOM | 3629 | O | LEU | B | 239 | 29.823 | 24.919 | 85.687 | 1.00 | 12.82 | O |
| ATOM | 3630 | CB | LEU | B | 239 | 28.325 | 24.020 | 83.092 | 1.00 | 12.97 | C |
| ATOM | 3631 | CG | LEU | B | 239 | 27.874 | 24.124 | 81.641 | 1.00 | 12.81 | C |
| ATOM | 3632 | CD1 | LEU | B | 239 | 28.202 | 22.836 | 80.913 | 1.00 | 10.97 | C |
| ATOM | 3633 | CD2 | LEU | B | 239 | 26.365 | 24.432 | 81.584 | 1.00 | 12.44 | C |
| ATOM | 3634 | N | PRO | B | 240 | 27.642 | 24.952 | 86.236 | 1.00 | 12.88 | N |
| ATOM | 3635 | CA | PRO | B | 240 | 27.869 | 24.819 | 87.688 | 1.00 | 12.68 | C |
| ATOM | 3636 | C | PRO | B | 240 | 28.288 | 23.416 | 88.106 | 1.00 | 13.42 | C |
| ATOM | 3637 | O | PRO | B | 240 | 28.120 | 22.485 | 87.319 | 1.00 | 14.52 | O |
| ATOM | 3638 | CB | PRO | B | 240 | 26.491 | 25.136 | 88.276 | 1.00 | 12.16 | C |
| ATOM | 3639 | CG | PRO | B | 240 | 25.533 | 24.665 | 87.217 | 1.00 | 11.29 | C |
| ATOM | 3640 | CD | PRO | B | 240 | 26.197 | 25.004 | 85.910 | 1.00 | 12.22 | C |
| ATOM | 3641 | N | GLN | B | 241 | 28.808 | 23.279 | 89.326 | 1.00 | 13.71 | N |
| ATOM | 3642 | CA | GLN | B | 241 | 29.254 | 22.000 | 89.879 | 1.00 | 14.12 | C |
| ATOM | 3643 | C | GLN | B | 241 | 28.063 | 21.103 | 90.199 | 1.00 | 14.23 | C |
| ATOM | 3644 | O | GLN | B | 241 | 27.214 | 21.480 | 91.005 | 1.00 | 15.16 | O |
| ATOM | 3645 | CB | GLN | B | 241 | 30.061 | 22.253 | 91.152 | 1.00 | 14.67 | C |
| ATOM | 3646 | CG | GLN | B | 241 | 30.628 | 21.019 | 91.861 | 1.00 | 14.50 | C |
| ATOM | 3647 | CD | GLN | B | 241 | 31.366 | 21.380 | 93.141 | 1.00 | 15.22 | C |
| ATOM | 3648 | OE1 | GLN | B | 241 | 31.656 | 22.551 | 93.390 | 1.00 | 17.17 | O |
| ATOM | 3649 | NE2 | GLN | B | 241 | 31.679 | 20.379 | 93.949 | 1.00 | 15.41 | N |
| ATOM | 3650 | N | PRO | B | 242 | 27.994 | 19.927 | 89.577 | 1.00 | 14.19 | N |
| ATOM | 3651 | CA | PRO | B | 242 | 26.899 | 18.985 | 89.845 | 1.00 | 14.08 | C |
| ATOM | 3652 | C | PRO | B | 242 | 26.889 | 18.561 | 91.310 | 1.00 | 13.95 | C |
| ATOM | 3653 | O | PRO | B | 242 | 27.968 | 18.432 | 91.894 | 1.00 | 15.61 | O |
| ATOM | 3654 | CB | PRO | B | 242 | 27.220 | 17.799 | 88.925 | 1.00 | 13.09 | C |

FIG. 5III

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3655 | CG | PRO | B | 242 | 28.074 | 18.402 | 87.846 | 1.00 | 13.75 | C |
| ATOM | 3656 | CD | PRO | B | 242 | 28.940 | 19.398 | 88.571 | 1.00 | 13.98 | C |
| ATOM | 3657 | N | PRO | B | 243 | 25.711 | 18.386 | 91.904 | 1.00 | 13.79 | N |
| ATOM | 3658 | CA | PRO | B | 243 | 25.603 | 17.963 | 93.308 | 1.00 | 13.77 | C |
| ATOM | 3659 | C | PRO | B | 243 | 26.433 | 16.721 | 93.663 | 1.00 | 14.39 | C |
| ATOM | 3660 | O | PRO | B | 243 | 26.956 | 16.657 | 94.786 | 1.00 | 14.49 | O |
| ATOM | 3661 | CB | PRO | B | 243 | 24.110 | 17.674 | 93.468 | 1.00 | 13.38 | C |
| ATOM | 3662 | CG | PRO | B | 243 | 23.452 | 18.564 | 92.473 | 1.00 | 13.06 | C |
| ATOM | 3663 | CD | PRO | B | 243 | 24.383 | 18.610 | 91.296 | 1.00 | 13.60 | C |
| ATOM | 3664 | N | ILE | B | 244 | 26.574 | 15.776 | 92.732 | 1.00 | 14.56 | N |
| ATOM | 3665 | CA | ILE | B | 244 | 27.276 | 14.513 | 93.021 | 1.00 | 15.32 | C |
| ATOM | 3666 | C | ILE | B | 244 | 28.793 | 14.614 | 92.881 | 1.00 | 15.58 | C |
| ATOM | 3667 | O | ILE | B | 244 | 29.523 | 13.705 | 93.302 | 1.00 | 16.52 | O |
| ATOM | 3668 | CB | ILE | B | 244 | 26.747 | 13.341 | 92.142 | 1.00 | 14.86 | C |
| ATOM | 3669 | CG1 | ILE | B | 244 | 27.265 | 13.462 | 90.694 | 1.00 | 15.57 | C |
| ATOM | 3670 | CD1 | ILE | B | 244 | 27.091 | 12.206 | 89.848 | 1.00 | 14.23 | C |
| ATOM | 3671 | CG2 | ILE | B | 244 | 25.217 | 13.248 | 92.220 | 1.00 | 14.47 | C |
| ATOM | 3672 | N | CYS | B | 245 | 29.267 | 15.706 | 92.289 | 1.00 | 15.23 | N |
| ATOM | 3673 | CA | CYS | B | 245 | 30.682 | 15.833 | 91.995 | 1.00 | 15.43 | C |
| ATOM | 3674 | C | CYS | B | 245 | 31.470 | 16.391 | 93.160 | 1.00 | 15.26 | C |
| ATOM | 3675 | O | CYS | B | 245 | 31.106 | 17.410 | 93.745 | 1.00 | 15.44 | O |
| ATOM | 3676 | CB | CYS | B | 245 | 30.911 | 16.717 | 90.770 | 1.00 | 15.92 | C |
| ATOM | 3677 | SG | CYS | B | 245 | 30.389 | 15.976 | 89.221 | 1.00 | 18.07 | S |
| ATOM | 3678 | N | THR | B | 246 | 32.565 | 15.720 | 93.492 | 1.00 | 14.87 | N |
| ATOM | 3679 | CA | THR | B | 246 | 33.587 | 16.353 | 94.306 | 1.00 | 14.14 | C |
| ATOM | 3680 | C | THR | B | 246 | 34.242 | 17.406 | 93.419 | 1.00 | 14.34 | C |
| ATOM | 3681 | O | THR | B | 246 | 34.088 | 17.379 | 92.179 | 1.00 | 14.25 | O |
| ATOM | 3682 | CB | THR | B | 246 | 34.629 | 15.335 | 94.806 | 1.00 | 14.14 | C |
| ATOM | 3683 | OG1 | THR | B | 246 | 35.186 | 14.629 | 93.691 | 1.00 | 13.28 | O |
| ATOM | 3684 | CG2 | THR | B | 246 | 33.958 | 14.251 | 95.643 | 1.00 | 12.79 | C |
| ATOM | 3685 | N | ILE | B | 247 | 34.954 | 18.335 | 94.045 | 1.00 | 13.78 | N |
| ATOM | 3686 | CA | ILE | B | 247 | 35.588 | 19.422 | 93.316 | 1.00 | 14.18 | C |
| ATOM | 3687 | C | ILE | B | 247 | 36.708 | 18.926 | 92.404 | 1.00 | 14.74 | C |
| ATOM | 3688 | O | ILE | B | 247 | 37.034 | 19.581 | 91.417 | 1.00 | 15.64 | O |
| ATOM | 3689 | CB | ILE | B | 247 | 36.086 | 20.542 | 94.300 | 1.00 | 14.39 | C |
| ATOM | 3690 | CG1 | ILE | B | 247 | 36.346 | 21.862 | 93.542 | 1.00 | 14.02 | C |
| ATOM | 3691 | CG2 | ILE | B | 247 | 37.291 | 20.069 | 95.113 | 1.00 | 12.39 | C |
| ATOM | 3692 | N | ASP | B | 248 | 37.287 | 17.771 | 92.727 | 1.00 | 15.22 | N |
| ATOM | 3693 | CA | ASP | B | 248 | 38.311 | 17.166 | 91.881 | 1.00 | 15.68 | C |
| ATOM | 3694 | C | ASP | B | 248 | 37.786 | 16.862 | 90.473 | 1.00 | 15.45 | C |
| ATOM | 3695 | O | ASP | B | 248 | 38.500 | 17.087 | 89.484 | 1.00 | 15.83 | O |
| ATOM | 3696 | CB | ASP | B | 248 | 38.871 | 15.905 | 92.530 | 1.00 | 16.79 | C |
| ATOM | 3697 | CG | ASP | B | 248 | 39.500 | 16.174 | 93.897 | 1.00 | 18.94 | C |
| ATOM | 3698 | OD1 | ASP | B | 248 | 38.815 | 16.723 | 94.791 | 1.00 | 21.19 | O |
| ATOM | 3699 | OD2 | ASP | B | 248 | 40.674 | 15.860 | 94.166 | 1.00 | 19.48 | O |
| ATOM | 3700 | N | VAL | B | 249 | 36.545 | 16.371 | 90.388 | 1.00 | 14.24 | N |
| ATOM | 3701 | CA | VAL | B | 249 | 35.926 | 16.013 | 89.106 | 1.00 | 13.40 | C |
| ATOM | 3702 | C | VAL | B | 249 | 35.535 | 17.266 | 88.329 | 1.00 | 13.20 | C |
| ATOM | 3703 | O | VAL | B | 249 | 35.783 | 17.369 | 87.126 | 1.00 | 12.26 | O |
| ATOM | 3704 | CB | VAL | B | 249 | 34.668 | 15.099 | 89.280 | 1.00 | 13.81 | C |
| ATOM | 3705 | CG1 | VAL | B | 249 | 34.045 | 14.760 | 87.915 | 1.00 | 13.08 | C |
| ATOM | 3706 | CG2 | VAL | B | 249 | 35.011 | 13.819 | 90.054 | 1.00 | 12.57 | C |
| ATOM | 3707 | N | TYR | B | 250 | 34.913 | 18.207 | 89.034 | 1.00 | 13.48 | N |
| ATOM | 3708 | CA | TYR | B | 250 | 34.542 | 19.506 | 88.479 | 1.00 | 13.90 | C |
| ATOM | 3709 | C | TYR | B | 250 | 35.733 | 20.286 | 87.906 | 1.00 | 14.58 | C |
| ATOM | 3710 | O | TYR | B | 250 | 35.614 | 20.900 | 86.850 | 1.00 | 14.68 | O |
| ATOM | 3711 | CB | TYR | B | 250 | 33.815 | 20.344 | 89.533 | 1.00 | 12.92 | C |
| ATOM | 3712 | CG | TYR | B | 250 | 33.230 | 21.645 | 89.005 | 1.00 | 11.54 | C |
| ATOM | 3713 | CD1 | TYR | B | 250 | 33.515 | 22.867 | 89.625 | 1.00 | 11.65 | C |
| ATOM | 3714 | CE1 | TYR | B | 250 | 32.974 | 24.055 | 89.154 | 1.00 | 11.22 | C |

FIG. 5JJJ

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3715 | CZ | TYR | B | 250 | 32.142 | 24.023 | 88.047 | 1.00 | 12.29 | C |
| ATOM | 3716 | OH | TYR | B | 250 | 31.582 | 25.189 | 87.558 | 1.00 | 12.34 | O |
| ATOM | 3717 | CE2 | TYR | B | 250 | 31.855 | 22.821 | 87.419 | 1.00 | 10.40 | C |
| ATOM | 3718 | CD2 | TYR | B | 250 | 32.396 | 21.650 | 87.903 | 1.00 | 10.00 | C |
| ATOM | 3719 | N | MET | B | 251 | 36.858 | 20.264 | 88.618 | 1.00 | 16.21 | N |
| ATOM | 3720 | CA | MET | B | 251 | 38.120 | 20.880 | 88.171 | 1.00 | 17.64 | C |
| ATOM | 3721 | C | MET | B | 251 | 38.581 | 20.391 | 86.785 | 1.00 | 17.75 | C |
| ATOM | 3722 | O | MET | B | 251 | 39.111 | 21.178 | 85.996 | 1.00 | 17.79 | O |
| ATOM | 3723 | CB | MET | B | 251 | 39.229 | 20.647 | 89.203 | 1.00 | 17.74 | C |
| ATOM | 3724 | CG | MET | B | 251 | 39.233 | 21.629 | 90.365 | 1.00 | 21.44 | C |
| ATOM | 3725 | SD | MET | B | 251 | 40.267 | 21.062 | 91.762 | 1.00 | 27.32 | S |
| ATOM | 3726 | CE | MET | B | 251 | 41.721 | 21.960 | 91.509 | 1.00 | 27.87 | C |
| ATOM | 3727 | N | ILE | B | 252 | 38.388 | 19.102 | 86.495 | 1.00 | 17.87 | N |
| ATOM | 3728 | CA | ILE | B | 252 | 38.654 | 18.574 | 85.152 | 1.00 | 18.51 | C |
| ATOM | 3729 | C | ILE | B | 252 | 37.730 | 19.186 | 84.108 | 1.00 | 18.27 | C |
| ATOM | 3730 | O | ILE | B | 252 | 38.181 | 19.544 | 83.013 | 1.00 | 18.74 | O |
| ATOM | 3731 | CB | ILE | B | 252 | 38.526 | 17.042 | 85.084 | 1.00 | 19.20 | C |
| ATOM | 3732 | CG1 | ILE | B | 252 | 39.443 | 16.370 | 86.093 | 1.00 | 20.17 | C |
| ATOM | 3733 | CD1 | ILE | B | 252 | 39.032 | 14.961 | 86.378 | 1.00 | 23.78 | C |
| ATOM | 3734 | CG2 | ILE | B | 252 | 38.873 | 16.549 | 83.682 | 1.00 | 19.28 | C |
| ATOM | 3735 | N | MET | B | 253 | 36.445 | 19.291 | 84.444 | 1.00 | 17.73 | N |
| ATOM | 3736 | CA | MET | B | 253 | 35.456 | 19.906 | 83.560 | 1.00 | 17.78 | C |
| ATOM | 3737 | C | MET | B | 253 | 35.860 | 21.346 | 83.224 | 1.00 | 17.74 | C |
| ATOM | 3738 | O | MET | B | 253 | 35.894 | 21.732 | 82.060 | 1.00 | 17.41 | O |
| ATOM | 3739 | CB | MET | B | 253 | 34.054 | 19.877 | 84.189 | 1.00 | 17.77 | C |
| ATOM | 3740 | CG | MET | B | 253 | 33.508 | 18.478 | 84.505 | 1.00 | 18.61 | C |
| ATOM | 3741 | SD | MET | B | 253 | 31.797 | 18.471 | 85.149 | 1.00 | 19.86 | S |
| ATOM | 3742 | CE | MET | B | 253 | 31.836 | 17.018 | 86.082 | 1.00 | 19.64 | C |
| ATOM | 3743 | N | VAL | B | 254 | 36.180 | 22.121 | 84.254 | 1.00 | 17.59 | N |
| ATOM | 3744 | CA | VAL | B | 254 | 36.503 | 23.544 | 84.112 | 1.00 | 17.73 | C |
| ATOM | 3745 | C | VAL | B | 254 | 37.706 | 23.743 | 83.194 | 1.00 | 17.23 | C |
| ATOM | 3746 | O | VAL | B | 254 | 37.731 | 24.657 | 82.364 | 1.00 | 17.29 | O |
| ATOM | 3747 | CB | VAL | B | 254 | 36.748 | 24.199 | 85.506 | 1.00 | 17.93 | C |
| ATOM | 3748 | CG1 | VAL | B | 254 | 37.495 | 25.528 | 85.380 | 1.00 | 18.54 | C |
| ATOM | 3749 | CG2 | VAL | B | 254 | 35.419 | 24.376 | 86.260 | 1.00 | 17.08 | C |
| ATOM | 3750 | N | LYS | B | 255 | 38.687 | 22.859 | 83.343 | 1.00 | 17.16 | N |
| ATOM | 3751 | CA | LYS | B | 255 | 39.880 | 22.836 | 82.506 | 1.00 | 16.61 | C |
| ATOM | 3752 | C | LYS | B | 255 | 39.512 | 22.684 | 81.032 | 1.00 | 15.72 | C |
| ATOM | 3753 | O | LYS | B | 255 | 40.207 | 23.208 | 80.166 | 1.00 | 16.37 | O |
| ATOM | 3754 | CB | LYS | B | 255 | 40.802 | 21.691 | 82.947 | 1.00 | 17.11 | C |
| ATOM | 3755 | CG | LYS | B | 255 | 41.818 | 22.054 | 84.028 | 1.00 | 18.64 | C |
| ATOM | 3756 | CD | LYS | B | 255 | 42.103 | 20.882 | 84.970 | 1.00 | 19.39 | C |
| ATOM | 3757 | CE | LYS | B | 255 | 43.506 | 20.349 | 84.788 | 1.00 | 21.72 | C |
| ATOM | 3758 | NZ | LYS | B | 255 | 44.190 | 20.115 | 86.100 | 1.00 | 22.15 | N |
| ATOM | 3759 | N | CYS | B | 256 | 38.423 | 21.969 | 80.752 | 1.00 | 14.38 | N |
| ATOM | 3760 | CA | CYS | B | 256 | 37.957 | 21.761 | 79.381 | 1.00 | 14.28 | C |
| ATOM | 3761 | C | CYS | B | 256 | 37.374 | 23.023 | 78.742 | 1.00 | 14.34 | C |
| ATOM | 3762 | O | CYS | B | 256 | 37.261 | 23.102 | 77.518 | 1.00 | 14.06 | O |
| ATOM | 3763 | CB | CYS | B | 256 | 36.911 | 20.647 | 79.317 | 1.00 | 13.80 | C |
| ATOM | 3764 | SG | CYS | B | 256 | 37.547 | 18.985 | 79.618 | 1.00 | 14.32 | S |
| ATOM | 3765 | N | TRP | B | 257 | 37.004 | 23.988 | 79.580 | 1.00 | 13.91 | N |
| ATOM | 3766 | CA | TRP | B | 257 | 36.295 | 25.194 | 79.157 | 1.00 | 13.77 | C |
| ATOM | 3767 | C | TRP | B | 257 | 37.165 | 26.465 | 79.220 | 1.00 | 15.02 | C |
| ATOM | 3768 | O | TRP | B | 257 | 36.648 | 27.584 | 79.167 | 1.00 | 14.41 | O |
| ATOM | 3769 | CB | TRP | B | 257 | 35.042 | 25.383 | 80.023 | 1.00 | 12.55 | C |
| ATOM | 3770 | CG | TRP | B | 257 | 34.140 | 24.193 | 80.049 | 1.00 | 9.07 | C |
| ATOM | 3771 | CD1 | TRP | B | 257 | 33.892 | 23.342 | 79.019 | 1.00 | 5.44 | C |
| ATOM | 3772 | NE1 | TRP | B | 257 | 32.998 | 22.380 | 79.409 | 1.00 | 6.93 | N |
| ATOM | 3773 | CE2 | TRP | B | 257 | 32.643 | 22.594 | 80.715 | 1.00 | 7.17 | C |
| ATOM | 3774 | CD2 | TRP | B | 257 | 33.338 | 23.739 | 81.151 | 1.00 | 7.71 | C |

FIG. 5KKK

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3775 | CE3 | TRP | B | 257 | 33.136 | 24.186 | 82.473 | 1.00 | 8.05 | C |
| ATOM | 3776 | CZ3 | TRP | B | 257 | 32.261 | 23.477 | 83.304 | 1.00 | 6.27 | C |
| ATOM | 3777 | CH2 | TRP | B | 257 | 31.588 | 22.337 | 82.834 | 1.00 | 6.51 | C |
| ATOM | 3778 | CZ2 | TRP | B | 257 | 31.766 | 21.882 | 81.544 | 1.00 | 7.14 | C |
| ATOM | 3779 | N | MET | B | 258 | 38.478 | 26.292 | 79.334 | 1.00 | 16.06 | N |
| ATOM | 3780 | CA | MET | B | 258 | 39.384 | 27.428 | 79.285 | 1.00 | 18.60 | C |
| ATOM | 3781 | C | MET | B | 258 | 39.374 | 28.045 | 77.888 | 1.00 | 19.06 | C |
| ATOM | 3782 | O | MET | B | 258 | 39.352 | 27.323 | 76.892 | 1.00 | 20.11 | O |
| ATOM | 3783 | CB | MET | B | 258 | 40.794 | 27.020 | 79.714 | 1.00 | 18.90 | C |
| ATOM | 3784 | CG | MET | B | 258 | 40.945 | 26.949 | 81.224 | 1.00 | 21.95 | C |
| ATOM | 3785 | SD | MET | B | 258 | 42.402 | 26.035 | 81.734 | 1.00 | 30.27 | S |
| ATOM | 3786 | CE | MET | B | 258 | 42.043 | 25.815 | 83.408 | 1.00 | 27.94 | C |
| ATOM | 3787 | N | ILE | B | 259 | 39.367 | 29.376 | 77.817 | 1.00 | 19.93 | N |
| ATOM | 3788 | CA | ILE | B | 259 | 39.271 | 30.074 | 76.531 | 1.00 | 20.24 | C |
| ATOM | 3789 | C | ILE | B | 259 | 40.439 | 29.714 | 75.623 | 1.00 | 20.46 | C |
| ATOM | 3790 | O | ILE | B | 259 | 40.249 | 29.553 | 74.423 | 1.00 | 20.89 | O |
| ATOM | 3791 | CB | ILE | B | 259 | 39.151 | 31.609 | 76.719 | 1.00 | 20.93 | C |
| ATOM | 3792 | CG1 | ILE | B | 259 | 37.884 | 31.970 | 77.493 | 1.00 | 21.43 | C |
| ATOM | 3793 | CD1 | ILE | B | 259 | 36.577 | 31.480 | 76.863 | 1.00 | 23.32 | C |
| ATOM | 3794 | CG2 | ILE | B | 259 | 39.156 | 32.355 | 75.359 | 1.00 | 21.81 | C |
| ATOM | 3795 | N | ASP | B | 260 | 41.636 | 29.573 | 76.194 | 1.00 | 20.65 | N |
| ATOM | 3796 | CA | ASP | B | 260 | 42.797 | 29.173 | 75.414 | 1.00 | 20.93 | C |
| ATOM | 3797 | C | ASP | B | 260 | 42.796 | 27.662 | 75.198 | 1.00 | 21.14 | C |
| ATOM | 3798 | O | ASP | B | 260 | 43.024 | 26.889 | 76.126 | 1.00 | 20.65 | O |
| ATOM | 3799 | CB | ASP | B | 260 | 44.106 | 29.630 | 76.071 | 1.00 | 21.15 | C |
| ATOM | 3800 | CG | ASP | B | 260 | 45.321 | 29.442 | 75.160 | 1.00 | 22.12 | C |
| ATOM | 3801 | OD1 | ASP | B | 260 | 46.226 | 30.305 | 75.178 | 1.00 | 23.82 | O |
| ATOM | 3802 | OD2 | ASP | B | 260 | 45.460 | 28.470 | 74.386 | 1.00 | 22.28 | O |
| ATOM | 3803 | N | ALA | B | 261 | 42.556 | 27.269 | 73.951 | 1.00 | 21.77 | N |
| ATOM | 3804 | CA | ALA | B | 261 | 42.445 | 25.875 | 73.539 | 1.00 | 22.35 | C |
| ATOM | 3805 | C | ALA | B | 261 | 43.666 | 25.045 | 73.940 | 1.00 | 23.20 | C |
| ATOM | 3806 | O | ALA | B | 261 | 43.546 | 23.850 | 74.242 | 1.00 | 22.79 | O |
| ATOM | 3807 | CB | ALA | B | 261 | 42.217 | 25.802 | 72.036 | 1.00 | 21.66 | C |
| ATOM | 3808 | N | ASP | B | 262 | 44.829 | 25.694 | 73.958 | 1.00 | 24.00 | N |
| ATOM | 3809 | CA | ASP | B | 262 | 46.083 | 25.043 | 74.329 | 1.00 | 24.82 | C |
| ATOM | 3810 | C | ASP | B | 262 | 46.217 | 24.807 | 75.831 | 1.00 | 24.77 | C |
| ATOM | 3811 | O | ASP | B | 262 | 47.012 | 23.971 | 76.255 | 1.00 | 25.09 | O |
| ATOM | 3812 | CB | ASP | B | 262 | 47.278 | 25.833 | 73.784 | 1.00 | 25.21 | C |
| ATOM | 3813 | CG | ASP | B | 262 | 47.359 | 25.783 | 72.270 | 1.00 | 26.70 | C |
| ATOM | 3814 | OD1 | ASP | B | 262 | 47.079 | 24.712 | 71.693 | 1.00 | 28.08 | O |
| ATOM | 3815 | OD2 | ASP | B | 262 | 47.688 | 26.758 | 71.564 | 1.00 | 29.43 | O |
| ATOM | 3816 | N | SER | B | 263 | 45.447 | 25.553 | 76.623 | 1.00 | 24.81 | N |
| ATOM | 3817 | CA | SER | B | 263 | 45.372 | 25.362 | 78.071 | 1.00 | 24.47 | C |
| ATOM | 3818 | C | SER | B | 263 | 44.509 | 24.149 | 78.456 | 1.00 | 23.99 | C |
| ATOM | 3819 | O | SER | B | 263 | 44.596 | 23.661 | 79.580 | 1.00 | 24.56 | O |
| ATOM | 3820 | CB | SER | B | 263 | 44.796 | 26.612 | 78.744 | 1.00 | 24.66 | C |
| ATOM | 3821 | OG | SER | B | 263 | 45.670 | 27.720 | 78.626 | 1.00 | 26.51 | O |
| ATOM | 3822 | N | ARG | B | 264 | 43.658 | 23.696 | 77.537 | 1.00 | 22.96 | N |
| ATOM | 3823 | CA | ARG | B | 264 | 42.748 | 22.582 | 77.792 | 1.00 | 22.04 | C |
| ATOM | 3824 | C | ARG | B | 264 | 43.495 | 21.255 | 77.820 | 1.00 | 21.62 | C |
| ATOM | 3825 | O | ARG | B | 264 | 44.472 | 21.074 | 77.083 | 1.00 | 21.63 | O |
| ATOM | 3826 | CB | ARG | B | 264 | 41.669 | 22.512 | 76.708 | 1.00 | 22.15 | C |
| ATOM | 3827 | CG | ARG | B | 264 | 40.656 | 23.648 | 76.734 | 1.00 | 21.27 | C |
| ATOM | 3828 | CD | ARG | B | 264 | 39.725 | 23.679 | 75.532 | 1.00 | 18.87 | C |
| ATOM | 3829 | NE | ARG | B | 264 | 39.303 | 25.041 | 75.234 | 1.00 | 18.42 | N |
| ATOM | 3830 | CZ | ARG | B | 264 | 38.856 | 25.459 | 74.057 | 1.00 | 19.86 | C |
| ATOM | 3831 | NH1 | ARG | B | 264 | 38.512 | 26.730 | 73.909 | 1.00 | 19.76 | N |
| ATOM | 3832 | NH2 | ARG | B | 264 | 38.740 | 24.618 | 73.027 | 1.00 | 20.18 | N |
| ATOM | 3833 | N | PRO | B | 265 | 43.035 | 20.324 | 78.658 | 1.00 | 20.99 | N |
| ATOM | 3834 | CA | PRO | B | 265 | 43.554 | 18.952 | 78.640 | 1.00 | 20.37 | C |

FIG. 5LLL

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3835 | C | PRO | B | 265 | 43.422 | 18.352 | 77.248 | 1.00 | 20.21 | C |
| ATOM | 3836 | O | PRO | B | 265 | 42.597 | 18.807 | 76.451 | 1.00 | 20.47 | O |
| ATOM | 3837 | CB | PRO | B | 265 | 42.624 | 18.195 | 79.599 | 1.00 | 20.50 | C |
| ATOM | 3838 | CG | PRO | B | 265 | 41.892 | 19.223 | 80.399 | 1.00 | 20.26 | C |
| ATOM | 3839 | CD | PRO | B | 265 | 41.985 | 20.518 | 79.675 | 1.00 | 20.58 | C |
| ATOM | 3840 | N | LYS | B | 266 | 44.243 | 17.348 | 76.959 | 1.00 | 19.85 | N |
| ATOM | 3841 | CA | LYS | B | 266 | 44.143 | 16.588 | 75.724 | 1.00 | 18.81 | C |
| ATOM | 3842 | C | LYS | B | 266 | 43.412 | 15.300 | 76.067 | 1.00 | 18.67 | C |
| ATOM | 3843 | O | LYS | B | 266 | 43.386 | 14.908 | 77.236 | 1.00 | 18.91 | O |
| ATOM | 3844 | CB | LYS | B | 266 | 45.542 | 16.290 | 75.181 | 1.00 | 19.50 | C |
| ATOM | 3845 | CG | LYS | B | 266 | 46.300 | 17.529 | 74.654 | 1.00 | 18.95 | C |
| ATOM | 3846 | N | PHE | B | 267 | 42.821 | 14.634 | 75.075 | 1.00 | 17.83 | N |
| ATOM | 3847 | CA | PHE | B | 267 | 42.064 | 13.410 | 75.358 | 1.00 | 17.53 | C |
| ATOM | 3848 | C | PHE | B | 267 | 42.879 | 12.317 | 76.080 | 1.00 | 17.68 | C |
| ATOM | 3849 | O | PHE | B | 267 | 42.378 | 11.690 | 77.008 | 1.00 | 18.05 | O |
| ATOM | 3850 | CB | PHE | B | 267 | 41.351 | 12.877 | 74.103 | 1.00 | 16.96 | C |
| ATOM | 3851 | CG | PHE | B | 267 | 40.111 | 13.665 | 73.724 | 1.00 | 14.86 | C |
| ATOM | 3852 | CD1 | PHE | B | 267 | 39.015 | 13.725 | 74.581 | 1.00 | 11.46 | C |
| ATOM | 3853 | CE1 | PHE | B | 267 | 37.884 | 14.437 | 74.241 | 1.00 | 11.98 | C |
| ATOM | 3854 | CZ | PHE | B | 267 | 37.831 | 15.118 | 73.031 | 1.00 | 12.05 | C |
| ATOM | 3855 | CE2 | PHE | B | 267 | 38.915 | 15.073 | 72.169 | 1.00 | 12.75 | C |
| ATOM | 3856 | CD2 | PHE | B | 267 | 40.051 | 14.349 | 72.519 | 1.00 | 13.19 | C |
| ATOM | 3857 | N | ARG | B | 268 | 44.132 | 12.121 | 75.680 | 1.00 | 17.72 | N |
| ATOM | 3858 | CA | ARG | B | 268 | 45.047 | 11.207 | 76.380 | 1.00 | 18.48 | C |
| ATOM | 3859 | C | ARG | B | 268 | 45.182 | 11.529 | 77.879 | 1.00 | 18.44 | C |
| ATOM | 3860 | O | ARG | B | 268 | 45.247 | 10.630 | 78.720 | 1.00 | 19.38 | O |
| ATOM | 3861 | CB | ARG | B | 268 | 46.434 | 11.212 | 75.713 | 1.00 | 17.82 | C |
| ATOM | 3862 | N | GLU | B | 269 | 45.217 | 12.812 | 78.206 | 1.00 | 18.65 | N |
| ATOM | 3863 | CA | GLU | B | 269 | 45.297 | 13.250 | 79.597 | 1.00 | 18.92 | C |
| ATOM | 3864 | C | GLU | B | 269 | 43.959 | 13.036 | 80.322 | 1.00 | 18.54 | C |
| ATOM | 3865 | O | GLU | B | 269 | 43.934 | 12.647 | 81.497 | 1.00 | 18.09 | O |
| ATOM | 3866 | CB | GLU | B | 269 | 45.775 | 14.704 | 79.666 | 1.00 | 19.47 | C |
| ATOM | 3867 | CG | GLU | B | 269 | 46.966 | 14.979 | 78.738 | 1.00 | 21.92 | C |
| ATOM | 3868 | CD | GLU | B | 269 | 47.419 | 16.436 | 78.690 | 1.00 | 24.77 | C |
| ATOM | 3869 | OE1 | GLU | B | 269 | 46.571 | 17.354 | 78.653 | 1.00 | 24.51 | O |
| ATOM | 3870 | OE2 | GLU | B | 269 | 48.649 | 16.667 | 78.662 | 1.00 | 28.26 | O |
| ATOM | 3871 | N | LEU | B | 270 | 42.856 | 13.257 | 79.601 | 1.00 | 17.64 | N |
| ATOM | 3872 | CA | LEU | B | 270 | 41.514 | 12.934 | 80.102 | 1.00 | 16.64 | C |
| ATOM | 3873 | C | LEU | B | 270 | 41.332 | 11.431 | 80.367 | 1.00 | 16.54 | C |
| ATOM | 3874 | O | LEU | B | 270 | 40.745 | 11.052 | 81.385 | 1.00 | 16.13 | O |
| ATOM | 3875 | CB | LEU | B | 270 | 40.421 | 13.477 | 79.167 | 1.00 | 15.75 | C |
| ATOM | 3876 | CG | LEU | B | 270 | 40.365 | 15.011 | 79.069 | 1.00 | 15.92 | C |
| ATOM | 3877 | CD1 | LEU | B | 270 | 39.468 | 15.471 | 77.940 | 1.00 | 14.68 | C |
| ATOM | 3878 | CD2 | LEU | B | 270 | 39.927 | 15.641 | 80.380 | 1.00 | 15.30 | C |
| ATOM | 3879 | N | ILE | B | 271 | 41.844 | 10.581 | 79.472 | 1.00 | 16.42 | N |
| ATOM | 3880 | CA | ILE | B | 271 | 41.879 | 9.130 | 79.728 | 1.00 | 16.73 | C |
| ATOM | 3881 | C | ILE | B | 271 | 42.555 | 8.821 | 81.078 | 1.00 | 17.15 | C |
| ATOM | 3882 | O | ILE | B | 271 | 41.987 | 8.122 | 81.918 | 1.00 | 17.53 | O |
| ATOM | 3883 | CB | ILE | B | 271 | 42.560 | 8.346 | 78.550 | 1.00 | 16.37 | C |
| ATOM | 3884 | CG1 | ILE | B | 271 | 41.714 | 8.454 | 77.273 | 1.00 | 16.54 | C |
| ATOM | 3885 | CD1 | ILE | B | 271 | 42.422 | 8.022 | 75.984 | 1.00 | 15.02 | C |
| ATOM | 3886 | CG2 | ILE | B | 271 | 42.723 | 6.872 | 78.902 | 1.00 | 15.63 | C |
| ATOM | 3887 | N | ILE | B | 272 | 43.743 | 9.384 | 81.294 | 1.00 | 17.68 | N |
| ATOM | 3888 | CA | ILE | B | 272 | 44.536 | 9.127 | 82.505 | 1.00 | 18.08 | C |
| ATOM | 3889 | C | ILE | B | 272 | 43.816 | 9.599 | 83.774 | 1.00 | 18.08 | C |
| ATOM | 3890 | O | ILE | B | 272 | 43.737 | 8.875 | 84.764 | 1.00 | 17.54 | O |
| ATOM | 3891 | CB | ILE | B | 272 | 45.969 | 9.745 | 82.360 | 1.00 | 18.32 | C |
| ATOM | 3892 | CG1 | ILE | B | 272 | 46.789 | 8.931 | 81.355 | 1.00 | 18.63 | C |
| ATOM | 3893 | CD1 | ILE | B | 272 | 47.871 | 9.740 | 80.611 | 1.00 | 20.26 | C |
| ATOM | 3894 | CG2 | ILE | B | 272 | 46.704 | 9.861 | 83.716 | 1.00 | 17.93 | C |

FIG. 5MMM

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3895 | N | GLU | B | 273 | 43.255 | 10.798 | 83.715 | 1.00 | 18.86 | N |
| ATOM | 3896 | CA | GLU | B | 273 | 42.579 | 11.397 | 84.863 | 1.00 | 19.99 | C |
| ATOM | 3897 | C | GLU | B | 273 | 41.308 | 10.631 | 85.284 | 1.00 | 19.72 | C |
| ATOM | 3898 | O | GLU | B | 273 | 41.127 | 10.307 | 86.458 | 1.00 | 19.89 | O |
| ATOM | 3899 | CB | GLU | B | 273 | 42.278 | 12.864 | 84.565 | 1.00 | 21.15 | C |
| ATOM | 3900 | CG | GLU | B | 273 | 42.170 | 13.788 | 85.775 | 1.00 | 25.51 | C |
| ATOM | 3901 | CD | GLU | B | 273 | 43.171 | 13.489 | 86.872 | 1.00 | 28.87 | C |
| ATOM | 3902 | OE1 | GLU | B | 273 | 42.733 | 13.225 | 88.011 | 1.00 | 31.06 | O |
| ATOM | 3903 | OE2 | GLU | B | 273 | 44.390 | 13.514 | 86.602 | 1.00 | 31.27 | O |
| ATOM | 3904 | N | PHE | B | 274 | 40.452 | 10.304 | 84.323 | 1.00 | 19.07 | N |
| ATOM | 3905 | CA | PHE | B | 274 | 39.230 | 9.578 | 84.632 | 1.00 | 18.15 | C |
| ATOM | 3906 | C | PHE | B | 274 | 39.447 | 8.089 | 84.965 | 1.00 | 18.34 | C |
| ATOM | 3907 | O | PHE | B | 274 | 38.716 | 7.536 | 85.782 | 1.00 | 17.55 | O |
| ATOM | 3908 | CB | PHE | B | 274 | 38.198 | 9.779 | 83.523 | 1.00 | 17.98 | C |
| ATOM | 3909 | CG | PHE | B | 274 | 37.449 | 11.079 | 83.624 | 1.00 | 16.13 | C |
| ATOM | 3910 | CD1 | PHE | B | 274 | 36.467 | 11.258 | 84.594 | 1.00 | 16.35 | C |
| ATOM | 3911 | CE1 | PHE | B | 274 | 35.776 | 12.462 | 84.696 | 1.00 | 16.05 | C |
| ATOM | 3912 | CZ | PHE | B | 274 | 36.068 | 13.501 | 83.811 | 1.00 | 14.97 | C |
| ATOM | 3913 | CE2 | PHE | B | 274 | 37.052 | 13.333 | 82.853 | 1.00 | 14.62 | C |
| ATOM | 3914 | CD2 | PHE | B | 274 | 37.733 | 12.127 | 82.761 | 1.00 | 15.34 | C |
| ATOM | 3915 | N | SER | B | 275 | 40.443 | 7.451 | 84.341 | 1.00 | 18.52 | N |
| ATOM | 3916 | CA | SER | B | 275 | 40.821 | 6.071 | 84.683 | 1.00 | 18.91 | C |
| ATOM | 3917 | C | SER | B | 275 | 41.180 | 5.949 | 86.172 | 1.00 | 19.17 | C |
| ATOM | 3918 | O | SER | B | 275 | 40.699 | 5.057 | 86.866 | 1.00 | 18.84 | O |
| ATOM | 3919 | CB | SER | B | 275 | 42.007 | 5.593 | 83.832 | 1.00 | 19.09 | C |
| ATOM | 3920 | OG | SER | B | 275 | 41.668 | 5.439 | 82.463 | 1.00 | 19.74 | O |
| ATOM | 3921 | N | LYS | B | 276 | 42.028 | 6.862 | 86.636 | 1.00 | 19.68 | N |
| ATOM | 3922 | CA | LYS | B | 276 | 42.435 | 6.973 | 88.035 | 1.00 | 20.80 | C |
| ATOM | 3923 | C | LYS | B | 276 | 41.226 | 7.129 | 88.969 | 1.00 | 20.51 | C |
| ATOM | 3924 | O | LYS | B | 276 | 41.137 | 6.472 | 90.008 | 1.00 | 20.41 | O |
| ATOM | 3925 | CB | LYS | B | 276 | 43.400 | 8.160 | 88.176 | 1.00 | 21.66 | C |
| ATOM | 3926 | CG | LYS | B | 276 | 43.808 | 8.538 | 89.595 | 1.00 | 24.15 | C |
| ATOM | 3927 | CD | LYS | B | 276 | 45.169 | 9.248 | 89.638 | 1.00 | 27.89 | C |
| ATOM | 3928 | CE | LYS | B | 276 | 45.520 | 9.965 | 88.330 | 1.00 | 31.05 | C |
| ATOM | 3929 | NZ | LYS | B | 276 | 44.875 | 11.319 | 88.224 | 1.00 | 33.09 | N |
| ATOM | 3930 | N | MET | B | 277 | 40.292 | 7.985 | 88.572 | 1.00 | 20.28 | N |
| ATOM | 3931 | CA | MET | B | 277 | 39.066 | 8.219 | 89.333 | 1.00 | 19.77 | C |
| ATOM | 3932 | C | MET | B | 277 | 38.148 | 7.007 | 89.361 | 1.00 | 19.10 | C |
| ATOM | 3933 | O | MET | B | 277 | 37.528 | 6.717 | 90.386 | 1.00 | 18.35 | O |
| ATOM | 3934 | CB | MET | B | 277 | 38.332 | 9.430 | 88.772 | 1.00 | 20.05 | C |
| ATOM | 3935 | CG | MET | B | 277 | 39.095 | 10.718 | 88.997 | 1.00 | 20.14 | C |
| ATOM | 3936 | SD | MET | B | 277 | 38.213 | 12.164 | 88.415 | 1.00 | 22.55 | S |
| ATOM | 3937 | CE | MET | B | 277 | 39.128 | 13.416 | 89.378 | 1.00 | 20.86 | C |
| ATOM | 3938 | N | ALA | B | 278 | 38.093 | 6.297 | 88.236 | 1.00 | 18.93 | N |
| ATOM | 3939 | CA | ALA | B | 278 | 37.301 | 5.078 | 88.089 | 1.00 | 19.00 | C |
| ATOM | 3940 | C | ALA | B | 278 | 37.819 | 3.920 | 88.945 | 1.00 | 18.84 | C |
| ATOM | 3941 | O | ALA | B | 278 | 37.104 | 2.945 | 89.168 | 1.00 | 19.48 | O |
| ATOM | 3942 | CB | ALA | B | 278 | 37.238 | 4.663 | 86.626 | 1.00 | 19.11 | C |
| ATOM | 3943 | N | ARG | B | 279 | 39.060 | 4.026 | 89.413 | 1.00 | 18.31 | N |
| ATOM | 3944 | CA | ARG | B | 279 | 39.620 | 3.043 | 90.338 | 1.00 | 18.31 | C |
| ATOM | 3945 | C | ARG | B | 279 | 39.111 | 3.272 | 91.761 | 1.00 | 18.15 | C |
| ATOM | 3946 | O | ARG | B | 279 | 39.195 | 2.389 | 92.606 | 1.00 | 18.96 | O |
| ATOM | 3947 | CB | ARG | B | 279 | 41.146 | 3.100 | 90.326 | 1.00 | 18.23 | C |
| ATOM | 3948 | CG | ARG | B | 279 | 41.805 | 2.512 | 89.079 | 1.00 | 17.47 | C |
| ATOM | 3949 | CD | ARG | B | 279 | 43.321 | 2.406 | 89.195 | 1.00 | 15.59 | C |
| ATOM | 3950 | N | ASP | B | 280 | 38.602 | 4.468 | 92.026 | 1.00 | 17.90 | N |
| ATOM | 3951 | CA | ASP | B | 280 | 38.070 | 4.799 | 93.337 | 1.00 | 17.35 | C |
| ATOM | 3952 | C | ASP | B | 280 | 36.833 | 5.694 | 93.211 | 1.00 | 16.86 | C |
| ATOM | 3953 | O | ASP | B | 280 | 36.835 | 6.828 | 93.695 | 1.00 | 16.39 | O |
| ATOM | 3954 | CB | ASP | B | 280 | 39.152 | 5.482 | 94.168 | 1.00 | 17.42 | C |

FIG. 5NNN

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3955 | CG | ASP | B | 280 | 38.722 | 5.721 | 95.592 | 1.00 | 17.58 | C |
| ATOM | 3956 | OD1 | ASP | B | 280 | 37.701 | 5.134 | 96.018 | 1.00 | 16.77 | O |
| ATOM | 3957 | OD2 | ASP | B | 280 | 39.342 | 6.480 | 96.355 | 1.00 | 18.66 | O |
| ATOM | 3958 | N | PRO | B | 281 | 35.776 | 5.183 | 92.581 | 1.00 | 16.74 | N |
| ATOM | 3959 | CA | PRO | B | 281 | 34.662 | 6.028 | 92.132 | 1.00 | 17.14 | C |
| ATOM | 3960 | C | PRO | B | 281 | 33.827 | 6.616 | 93.269 | 1.00 | 17.98 | C |
| ATOM | 3961 | O | PRO | B | 281 | 33.305 | 7.729 | 93.113 | 1.00 | 17.71 | O |
| ATOM | 3962 | CB | PRO | B | 281 | 33.816 | 5.071 | 91.287 | 1.00 | 16.17 | C |
| ATOM | 3963 | CG | PRO | B | 281 | 34.076 | 3.745 | 91.875 | 1.00 | 16.96 | C |
| ATOM | 3964 | CD | PRO | B | 281 | 35.539 | 3.762 | 92.263 | 1.00 | 17.02 | C |
| ATOM | 3965 | N | GLN | B | 282 | 33.722 | 5.895 | 94.387 | 1.00 | 18.55 | N |
| ATOM | 3966 | CA | GLN | B | 282 | 32.905 | 6.345 | 95.509 | 1.00 | 19.76 | C |
| ATOM | 3967 | C | GLN | B | 282 | 33.569 | 7.462 | 96.309 | 1.00 | 20.19 | C |
| ATOM | 3968 | O | GLN | B | 282 | 32.955 | 8.031 | 97.207 | 1.00 | 21.77 | O |
| ATOM | 3969 | CB | GLN | B | 282 | 32.492 | 5.169 | 96.409 | 1.00 | 20.07 | C |
| ATOM | 3970 | CG | GLN | B | 282 | 31.583 | 4.160 | 95.701 | 1.00 | 21.32 | C |
| ATOM | 3971 | CD | GLN | B | 282 | 31.110 | 3.038 | 96.606 | 1.00 | 23.46 | C |
| ATOM | 3972 | OE1 | GLN | B | 282 | 30.267 | 3.248 | 97.469 | 1.00 | 23.51 | O |
| ATOM | 3973 | NE2 | GLN | B | 282 | 31.642 | 1.838 | 96.398 | 1.00 | 25.50 | N |
| ATOM | 3974 | N | ARG | B | 283 | 34.814 | 7.787 | 95.983 | 1.00 | 20.08 | N |
| ATOM | 3975 | CA | ARG | B | 283 | 35.465 | 8.950 | 96.575 | 1.00 | 20.64 | C |
| ATOM | 3976 | C | ARG | B | 283 | 35.237 | 10.217 | 95.720 | 1.00 | 20.11 | C |
| ATOM | 3977 | O | ARG | B | 283 | 35.264 | 11.342 | 96.236 | 1.00 | 19.20 | O |
| ATOM | 3978 | CB | ARG | B | 283 | 36.964 | 8.685 | 96.761 | 1.00 | 21.20 | C |
| ATOM | 3979 | CG | ARG | B | 283 | 37.812 | 9.924 | 96.950 | 1.00 | 23.87 | C |
| ATOM | 3980 | CD | ARG | B | 283 | 39.147 | 9.854 | 96.258 | 1.00 | 29.31 | C |
| ATOM | 3981 | NE | ARG | B | 283 | 39.846 | 11.142 | 96.233 | 1.00 | 33.72 | N |
| ATOM | 3982 | CZ | ARG | B | 283 | 41.166 | 11.276 | 96.354 | 1.00 | 35.62 | C |
| ATOM | 3983 | NH1 | ARG | B | 283 | 41.935 | 10.205 | 96.525 | 1.00 | 36.82 | N |
| ATOM | 3984 | NH2 | ARG | B | 283 | 41.719 | 12.482 | 96.318 | 1.00 | 36.16 | N |
| ATOM | 3985 | N | TYR | B | 284 | 35.018 | 10.025 | 94.419 | 1.00 | 19.02 | N |
| ATOM | 3986 | CA | TYR | B | 284 | 34.991 | 11.146 | 93.484 | 1.00 | 19.17 | C |
| ATOM | 3987 | C | TYR | B | 284 | 33.587 | 11.647 | 93.173 | 1.00 | 19.39 | C |
| ATOM | 3988 | O | TYR | B | 284 | 33.400 | 12.809 | 92.794 | 1.00 | 19.17 | O |
| ATOM | 3989 | CB | TYR | B | 284 | 35.752 | 10.802 | 92.209 | 1.00 | 18.39 | C |
| ATOM | 3990 | CG | TYR | B | 284 | 37.235 | 10.810 | 92.427 | 1.00 | 17.96 | C |
| ATOM | 3991 | CD1 | TYR | B | 284 | 37.956 | 9.612 | 92.544 | 1.00 | 17.88 | C |
| ATOM | 3992 | CE1 | TYR | B | 284 | 39.335 | 9.622 | 92.757 | 1.00 | 16.67 | C |
| ATOM | 3993 | CZ | TYR | B | 284 | 39.992 | 10.841 | 92.866 | 1.00 | 17.31 | C |
| ATOM | 3994 | OH | TYR | B | 284 | 41.346 | 10.891 | 93.077 | 1.00 | 19.02 | O |
| ATOM | 3995 | CE2 | TYR | B | 284 | 39.300 | 12.031 | 92.767 | 1.00 | 17.06 | C |
| ATOM | 3996 | CD2 | TYR | B | 284 | 37.925 | 12.011 | 92.552 | 1.00 | 17.89 | C |
| ATOM | 3997 | N | LEU | B | 285 | 32.613 | 10.757 | 93.342 | 1.00 | 19.77 | N |
| ATOM | 3998 | CA | LEU | B | 285 | 31.206 | 11.088 | 93.172 | 1.00 | 20.32 | C |
| ATOM | 3999 | C | LEU | B | 285 | 30.413 | 10.630 | 94.390 | 1.00 | 20.52 | C |
| ATOM | 4000 | O | LEU | B | 285 | 30.627 | 9.535 | 94.910 | 1.00 | 20.32 | O |
| ATOM | 4001 | CB | LEU | B | 285 | 30.644 | 10.450 | 91.899 | 1.00 | 20.09 | C |
| ATOM | 4002 | CG | LEU | B | 285 | 31.270 | 10.900 | 90.577 | 1.00 | 20.18 | C |
| ATOM | 4003 | CD1 | LEU | B | 285 | 30.599 | 10.197 | 89.399 | 1.00 | 18.74 | C |
| ATOM | 4004 | CD2 | LEU | B | 285 | 31.191 | 12.425 | 90.436 | 1.00 | 20.43 | C |
| ATOM | 4005 | N | VAL | B | 286 | 29.515 | 11.491 | 94.841 | 1.00 | 20.74 | N |
| ATOM | 4006 | CA | VAL | B | 286 | 28.710 | 11.227 | 96.017 | 1.00 | 21.57 | C |
| ATOM | 4007 | C | VAL | B | 286 | 27.299 | 10.882 | 95.569 | 1.00 | 22.00 | C |
| ATOM | 4008 | O | VAL | B | 286 | 26.532 | 11.760 | 95.176 | 1.00 | 21.78 | O |
| ATOM | 4009 | CB | VAL | B | 286 | 28.666 | 12.443 | 96.979 | 1.00 | 21.93 | C |
| ATOM | 4010 | CG1 | VAL | B | 286 | 27.971 | 12.061 | 98.289 | 1.00 | 21.50 | C |
| ATOM | 4011 | CG2 | VAL | B | 286 | 30.057 | 12.981 | 97.242 | 1.00 | 20.81 | C |
| ATOM | 4012 | N | ILE | B | 287 | 26.982 | 9.592 | 95.620 | 1.00 | 22.91 | N |
| ATOM | 4013 | CA | ILE | B | 287 | 25.682 | 9.069 | 95.224 | 1.00 | 23.56 | C |
| ATOM | 4014 | C | ILE | B | 287 | 24.978 | 8.518 | 96.460 | 1.00 | 24.37 | C |

FIG. 5000

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| ATOM | 4015 | O | ILE | B | 287 | 25.566 | 7.749 | 97.227 | 1.00 | 24.24 | O |
| ATOM | 4016 | CB | ILE | B | 287 | 25.869 | 7.960 | 94.163 | 1.00 | 23.71 | C |
| ATOM | 4017 | CG1 | ILE | B | 287 | 26.848 | 8.417 | 93.056 | 1.00 | 24.45 | C |
| ATOM | 4018 | CD1 | ILE | B | 287 | 26.217 | 8.809 | 91.717 | 1.00 | 24.37 | C |
| ATOM | 4019 | CG2 | ILE | B | 287 | 24.522 | 7.464 | 93.640 | 1.00 | 22.87 | C |
| ATOM | 4020 | N | GLN | B | 288 | 23.720 | 8.911 | 96.649 | 1.00 | 25.68 | N |
| ATOM | 4021 | CA | GLN | B | 288 | 22.935 | 8.519 | 97.827 | 1.00 | 26.67 | C |
| ATOM | 4022 | C | GLN | B | 288 | 22.874 | 7.005 | 98.069 | 1.00 | 27.26 | C |
| ATOM | 4023 | O | GLN | B | 288 | 23.109 | 6.543 | 99.190 | 1.00 | 27.59 | O |
| ATOM | 4024 | CB | GLN | B | 288 | 21.513 | 9.073 | 97.718 | 1.00 | 27.30 | C |
| ATOM | 4025 | N | GLY | B | 289 | 22.561 | 6.241 | 97.023 | 1.00 | 27.43 | N |
| ATOM | 4026 | CA | GLY | B | 289 | 22.472 | 4.791 | 97.119 | 1.00 | 27.67 | C |
| ATOM | 4027 | C | GLY | B | 289 | 23.782 | 4.132 | 97.516 | 1.00 | 27.87 | C |
| ATOM | 4028 | O | GLY | B | 289 | 23.803 | 2.980 | 97.949 | 1.00 | 28.06 | O |
| ATOM | 4029 | N | GLU | B | 290 | 24.874 | 4.865 | 97.323 | 1.00 | 27.98 | N |
| ATOM | 4030 | CA | GLU | B | 290 | 26.174 | 4.533 | 97.891 | 1.00 | 28.19 | C |
| ATOM | 4031 | C | GLU | B | 290 | 26.252 | 5.344 | 99.187 | 1.00 | 28.28 | C |
| ATOM | 4032 | O | GLU | B | 290 | 25.465 | 6.261 | 99.398 | 1.00 | 29.39 | O |
| ATOM | 4033 | CB | GLU | B | 290 | 27.291 | 4.889 | 96.897 | 1.00 | 27.86 | C |
| ATOM | 4034 | CG | GLU | B | 290 | 27.085 | 4.233 | 95.529 | 1.00 | 27.75 | C |
| ATOM | 4035 | CD | GLU | B | 290 | 27.996 | 4.741 | 94.412 | 1.00 | 26.76 | C |
| ATOM | 4036 | OE1 | GLU | B | 290 | 28.759 | 5.713 | 94.598 | 1.00 | 27.18 | O |
| ATOM | 4037 | OE2 | GLU | B | 290 | 27.949 | 4.146 | 93.324 | 1.00 | 25.95 | O |
| ATOM | 4038 | N | GLY | B | 291 | 27.145 | 5.013 | 100.095 | 1.00 | 27.84 | N |
| ATOM | 4039 | CA | GLY | B | 291 | 27.055 | 5.679 | 101.387 | 1.00 | 27.67 | C |
| ATOM | 4040 | C | GLY | B | 291 | 26.039 | 5.026 | 102.317 | 1.00 | 26.84 | C |
| ATOM | 4041 | O | GLY | B | 291 | 25.172 | 4.273 | 101.886 | 1.00 | 26.95 | O |
| ATOM | 4042 | N | HIS | B | 292 | 26.144 | 5.337 | 103.600 | 1.00 | 26.59 | N |
| ATOM | 4043 | CA | HIS | B | 292 | 25.449 | 4.590 | 104.635 | 1.00 | 26.57 | C |
| ATOM | 4044 | C | HIS | B | 292 | 24.255 | 5.332 | 105.232 | 1.00 | 26.85 | C |
| ATOM | 4045 | O | HIS | B | 292 | 24.033 | 6.512 | 104.948 | 1.00 | 26.45 | O |
| ATOM | 4046 | CB | HIS | B | 292 | 26.446 | 4.220 | 105.732 | 1.00 | 26.27 | C |
| ATOM | 4047 | CG | HIS | B | 292 | 26.944 | 5.394 | 106.514 | 1.00 | 25.62 | C |
| ATOM | 4048 | ND1 | HIS | B | 292 | 28.228 | 5.878 | 106.393 | 1.00 | 25.87 | N |
| ATOM | 4049 | CE1 | HIS | B | 292 | 28.388 | 6.908 | 107.202 | 1.00 | 25.43 | C |
| ATOM | 4050 | NE2 | HIS | B | 292 | 27.249 | 7.115 | 107.839 | 1.00 | 26.23 | N |
| ATOM | 4051 | CD2 | HIS | B | 292 | 26.331 | 6.179 | 107.430 | 1.00 | 24.56 | C |
| ATOM | 4052 | N | HIS | B | 293 | 23.503 | 4.634 | 106.077 | 1.00 | 27.57 | N |
| ATOM | 4053 | CA | HIS | B | 293 | 22.318 | 5.207 | 106.718 | 1.00 | 28.31 | C |
| ATOM | 4054 | C | HIS | B | 293 | 22.485 | 5.339 | 108.237 | 1.00 | 28.96 | C |
| ATOM | 4055 | O | HIS | B | 293 | 21.591 | 4.958 | 109.012 | 1.00 | 28.94 | O |
| ATOM | 4056 | CB | HIS | B | 293 | 21.088 | 4.357 | 106.388 | 1.00 | 28.43 | C |
| ATOM | 4057 | N | HIS | B | 294 | 23.635 | 5.875 | 108.655 | 1.00 | 29.44 | N |
| ATOM | 4058 | CA | HIS | B | 294 | 23.952 | 6.066 | 110.074 | 1.00 | 29.99 | C |
| ATOM | 4059 | C | HIS | B | 294 | 24.705 | 7.370 | 110.290 | 1.00 | 30.49 | C |
| ATOM | 4060 | O | HIS | B | 294 | 25.869 | 7.372 | 110.702 | 1.00 | 30.87 | O |
| ATOM | 4061 | CB | HIS | B | 294 | 24.785 | 4.905 | 110.612 | 1.00 | 29.51 | C |
| ATOM | 4062 | CG | HIS | B | 294 | 24.199 | 3.559 | 110.332 | 1.00 | 29.56 | C |
| ATOM | 4063 | ND1 | HIS | B | 294 | 22.922 | 3.211 | 110.715 | 1.00 | 28.90 | N |
| ATOM | 4064 | CE1 | HIS | B | 294 | 22.675 | 1.972 | 110.329 | 1.00 | 29.26 | C |
| ATOM | 4065 | NE2 | HIS | B | 294 | 23.748 | 1.502 | 109.718 | 1.00 | 29.18 | N |
| ATOM | 4066 | CD2 | HIS | B | 294 | 24.717 | 2.474 | 109.708 | 1.00 | 28.78 | C |
| ATOM | 4067 | N | HIS | B | 295 | 24.043 | 8.479 | 109.992 | 1.00 | 30.81 | N |
| ATOM | 4068 | CA | HIS | B | 295 | 24.641 | 9.786 | 110.191 | 1.00 | 31.27 | C |
| ATOM | 4069 | C | HIS | B | 295 | 24.101 | 10.403 | 111.471 | 1.00 | 31.79 | C |
| ATOM | 4070 | O | HIS | B | 295 | 22.910 | 10.723 | 111.568 | 1.00 | 31.64 | O |
| ATOM | 4071 | CB | HIS | B | 295 | 24.382 | 10.685 | 108.978 | 1.00 | 31.22 | C |
| ATOM | 4072 | CG | HIS | B | 295 | 25.066 | 10.222 | 107.731 | 1.00 | 30.61 | C |
| ATOM | 4073 | ND1 | HIS | B | 295 | 26.382 | 10.522 | 107.449 | 1.00 | 31.05 | N |
| ATOM | 4074 | CE1 | HIS | B | 295 | 26.715 | 9.979 | 106.292 | 1.00 | 30.84 | C |

FIG. 5PPP

| | | | | | | | | | | | |
|--------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| ATOM | 4075 | NE2 | HIS | B | 295 | 25.666 | 9.331 | 105.818 | 1.00 | 30.64 | N |
| ATOM | 4076 | CD2 | HIS | B | 295 | 24.623 | 9.467 | 106.700 | 1.00 | 30.41 | C |
| ATOM | 4077 | N | HIS | B | 296 | 24.986 | 10.537 | 112.457 | 1.00 | 32.57 | N |
| ATOM | 4078 | CA | HIS | B | 296 | 24.641 | 11.108 | 113.755 | 1.00 | 33.22 | C |
| ATOM | 4079 | C | HIS | B | 296 | 25.464 | 12.369 | 114.009 | 1.00 | 33.60 | C |
| ATOM | 4080 | O | HIS | B | 296 | 25.440 | 13.310 | 113.205 | 1.00 | 33.93 | O |
| ATOM | 4081 | CB | HIS | B | 296 | 24.856 | 10.087 | 114.880 | 1.00 | 33.38 | C |
| ATOM | 4082 | CG | HIS | B | 296 | 24.010 | 8.859 | 114.754 | 1.00 | 33.96 | C |
| ATOM | 4083 | ND1 | HIS | B | 296 | 24.213 | 7.914 | 113.769 | 1.00 | 35.11 | N |
| ATOM | 4084 | CE1 | HIS | B | 296 | 23.319 | 6.949 | 113.897 | 1.00 | 35.18 | C |
| ATOM | 4085 | NE2 | HIS | B | 296 | 22.541 | 7.234 | 114.928 | 1.00 | 34.93 | N |
| ATOM | 4086 | CD2 | HIS | B | 296 | 22.952 | 8.424 | 115.480 | 1.00 | 34.60 | C |
| TER | 4087 | | HIS | B | 296 | | | | | | |
| HETATM | 4088 | O | HOH | W | 1 | 28.998 | 7.797 | 96.214 | 1.00 | 5.45 | O |
| HETATM | 4089 | O | HOH | W | 2 | 42.694 | 30.033 | 78.928 | 1.00 | 15.99 | O |
| HETATM | 4090 | O | HOH | W | 3 | 14.284 | 24.355 | -1.705 | 1.00 | 31.92 | O |
| HETATM | 4091 | O | HOH | W | 4 | 9.434 | 2.124 | 25.854 | 1.00 | 12.89 | O |
| HETATM | 4092 | O | HOH | W | 5 | 11.686 | 18.337 | 20.467 | 1.00 | 19.43 | O |
| HETATM | 4093 | O | HOH | W | 6 | 28.232 | 0.015 | 63.543 | 1.00 | 23.69 | O |
| HETATM | 4094 | O | HOH | W | 7 | 32.566 | 18.198 | 69.464 | 1.00 | 16.45 | O |
| HETATM | 4095 | O | HOH | W | 8 | 26.983 | 7.994 | 103.693 | 1.00 | 28.59 | O |
| HETATM | 4096 | O | HOH | W | 9 | 34.576 | 20.314 | 67.899 | 1.00 | 13.64 | O |
| HETATM | 4097 | O | HOH | W | 10 | 22.822 | 24.473 | 71.792 | 1.00 | 14.22 | O |
| HETATM | 4098 | O | HOH | W | 11 | 42.907 | 16.304 | 72.715 | 1.00 | 17.29 | O |
| HETATM | 4099 | O | HOH | W | 12 | 17.470 | 20.215 | 83.374 | 1.00 | 14.31 | O |
| HETATM | 4100 | O | HOH | W | 13 | 1.076 | 16.872 | 17.542 | 1.00 | 17.35 | O |
| HETATM | 4101 | O | HOH | W | 14 | 20.657 | 17.529 | 73.818 | 1.00 | 14.37 | O |
| HETATM | 4102 | O | HOH | W | 15 | 38.164 | 24.544 | 61.487 | 1.00 | 25.36 | O |
| HETATM | 4103 | O | HOH | W | 16 | 41.611 | 2.775 | 62.349 | 1.00 | 16.19 | O |
| HETATM | 4104 | O | HOH | W | 17 | 22.137 | 2.221 | 23.260 | 1.00 | 20.64 | O |
| HETATM | 4105 | O | HOH | W | 18 | 14.764 | 24.583 | 13.369 | 1.00 | 10.86 | O |
| HETATM | 4106 | O | HOH | W | 19 | 40.188 | 2.839 | 85.624 | 1.00 | 27.07 | O |
| HETATM | 4107 | O | HOH | W | 20 | 1.841 | 30.006 | 10.579 | 1.00 | 21.05 | O |
| HETATM | 4108 | O | HOH | W | 21 | 40.127 | 2.221 | 72.748 | 1.00 | 28.26 | O |
| HETATM | 4109 | O | HOH | W | 22 | 13.323 | 6.174 | -5.504 | 1.00 | 18.62 | O |
| HETATM | 4110 | O | HOH | W | 23 | 34.315 | 1.583 | 64.924 | 1.00 | 16.89 | O |
| HETATM | 4111 | O | HOH | W | 24 | 21.460 | 7.245 | 94.994 | 1.00 | 29.64 | O |
| HETATM | 4112 | O | HOH | W | 25 | -0.062 | 6.376 | 21.264 | 1.00 | 21.21 | O |
| HETATM | 4113 | O | HOH | W | 26 | 33.676 | -4.733 | 22.767 | 1.00 | 25.95 | O |
| HETATM | 4114 | O | HOH | W | 27 | 29.411 | 25.141 | 76.288 | 1.00 | 12.37 | O |
| HETATM | 4115 | O | HOH | W | 28 | 13.514 | 0.588 | 25.186 | 1.00 | 22.58 | O |
| HETATM | 4116 | O | HOH | W | 29 | 35.216 | 16.749 | 60.751 | 1.00 | 34.92 | O |
| HETATM | 4117 | O | HOH | W | 30 | 29.873 | 0.309 | 65.863 | 1.00 | 22.64 | O |
| HETATM | 4118 | O | HOH | W | 31 | 39.650 | 17.942 | 97.058 | 1.00 | 14.17 | O |
| HETATM | 4119 | O | HOH | W | 32 | 15.423 | 0.311 | 27.412 | 1.00 | 29.42 | O |
| HETATM | 4120 | O | HOH | W | 33 | 24.729 | 15.715 | 90.114 | 1.00 | 16.40 | O |
| HETATM | 4121 | O | HOH | W | 34 | 11.022 | 23.047 | 19.968 | 1.00 | 28.41 | O |
| HETATM | 4122 | O | HOH | W | 35 | 15.226 | 26.439 | 14.982 | 1.00 | 10.40 | O |
| HETATM | 4123 | O | HOH | W | 36 | 29.549 | 7.754 | 98.929 | 1.00 | 31.05 | O |
| HETATM | 4124 | O | HOH | W | 37 | 24.144 | 13.769 | 108.784 | 1.00 | 19.16 | O |
| HETATM | 4125 | O | HOH | W | 38 | 44.398 | 22.138 | 81.434 | 1.00 | 22.62 | O |
| HETATM | 4126 | O | HOH | W | 39 | 30.484 | 26.026 | 80.696 | 1.00 | 16.25 | O |
| HETATM | 4127 | O | HOH | W | 40 | 23.926 | 2.662 | 21.574 | 1.00 | 38.97 | O |
| HETATM | 4128 | O | HOH | W | 41 | 24.201 | 23.722 | 11.877 | 1.00 | 22.52 | O |
| HETATM | 4129 | O | HOH | W | 42 | 38.768 | 14.851 | 67.829 | 1.00 | 18.62 | O |
| HETATM | 4130 | O | HOH | W | 43 | 20.593 | 10.669 | 109.434 | 1.00 | 25.90 | O |
| HETATM | 4131 | O | HOH | W | 44 | 9.833 | 38.268 | 17.805 | 1.00 | 40.12 | O |
| HETATM | 4132 | O | HOH | W | 45 | 31.806 | 15.563 | 61.831 | 1.00 | 38.92 | O |
| HETATM | 4133 | O | HOH | W | 46 | 46.648 | 15.389 | 67.532 | 1.00 | 45.52 | O |
| HETATM | 4134 | O | HOH | W | 47 | 7.194 | 26.606 | 7.278 | 1.00 | 24.59 | O |

FIG. 5QQQ

| | | | | | | | | | | | |
|--------|------|---|-----|---|-----|--------|--------|---------|------|-------|---|
| HETATM | 4135 | O | HOH | W | 48 | 32.345 | 9.389 | 45.870 | 1.00 | 37.43 | O |
| HETATM | 4136 | O | HOH | W | 49 | 34.408 | -0.038 | 92.412 | 1.00 | 30.28 | O |
| HETATM | 4137 | O | HOH | W | 50 | 29.018 | 26.702 | 74.110 | 1.00 | 12.47 | O |
| HETATM | 4138 | O | HOH | W | 51 | 26.345 | 37.094 | 83.883 | 1.00 | 44.10 | O |
| HETATM | 4139 | O | HOH | W | 52 | 17.751 | 17.183 | 85.261 | 1.00 | 29.92 | O |
| HETATM | 4140 | O | HOH | W | 53 | 8.300 | 30.037 | 4.708 | 1.00 | 30.49 | O |
| HETATM | 4141 | O | HOH | W | 54 | 7.052 | 1.135 | -4.627 | 1.00 | 50.89 | O |
| HETATM | 4142 | O | HOH | W | 55 | 10.934 | 5.449 | 56.316 | 1.00 | 59.86 | O |
| HETATM | 4143 | O | HOH | W | 56 | 9.455 | 20.642 | 21.947 | 1.00 | 16.62 | O |
| HETATM | 4144 | O | HOH | W | 57 | 36.716 | 27.172 | 82.502 | 1.00 | 28.06 | O |
| HETATM | 4145 | O | HOH | W | 58 | 21.316 | 4.587 | 29.057 | 1.00 | 19.72 | O |
| HETATM | 4146 | O | HOH | W | 59 | 25.658 | 12.245 | 41.218 | 1.00 | 37.60 | O |
| HETATM | 4147 | O | HOH | W | 60 | 19.391 | 9.604 | 99.993 | 1.00 | 34.08 | O |
| HETATM | 4148 | O | HOH | W | 61 | 12.023 | 36.817 | 22.931 | 1.00 | 30.96 | O |
| HETATM | 4149 | O | HOH | W | 62 | 18.695 | 36.508 | 6.780 | 1.00 | 42.88 | O |
| HETATM | 4150 | O | HOH | W | 63 | 29.545 | 25.882 | 90.977 | 1.00 | 26.81 | O |
| HETATM | 4151 | O | HOH | W | 64 | 22.863 | 13.391 | 21.494 | 1.00 | 34.76 | O |
| HETATM | 4152 | O | HOH | W | 65 | 2.066 | 3.306 | 28.674 | 1.00 | 25.12 | O |
| HETATM | 4153 | O | HOH | W | 66 | 21.290 | 17.351 | 78.158 | 1.00 | 22.87 | O |
| HETATM | 4154 | O | HOH | W | 67 | 17.483 | 6.317 | 73.617 | 1.00 | 28.08 | O |
| HETATM | 4155 | O | HOH | W | 68 | 32.056 | 1.581 | 48.187 | 1.00 | 34.21 | O |
| HETATM | 4156 | O | HOH | W | 69 | 27.862 | 18.784 | 70.341 | 1.00 | 18.12 | O |
| HETATM | 4157 | O | HOH | W | 70 | 16.168 | 15.234 | 27.154 | 1.00 | 18.67 | O |
| HETATM | 4158 | O | HOH | W | 71 | 27.548 | -1.447 | 15.790 | 1.00 | 28.43 | O |
| HETATM | 4159 | O | HOH | W | 72 | -3.252 | 8.681 | 19.344 | 1.00 | 28.54 | O |
| HETATM | 4160 | O | HOH | W | 73 | 21.775 | 24.157 | 17.335 | 1.00 | 31.82 | O |
| HETATM | 4161 | O | HOH | W | 74 | 32.097 | -6.189 | 21.261 | 1.00 | 36.61 | O |
| HETATM | 4162 | O | HOH | W | 75 | 5.334 | 15.234 | 22.514 | 1.00 | 22.29 | O |
| HETATM | 4163 | O | HOH | W | 76 | 26.436 | 16.890 | 13.243 | 1.00 | 46.48 | O |
| HETATM | 4164 | O | HOH | W | 77 | 26.507 | 8.991 | 99.475 | 1.00 | 28.94 | O |
| HETATM | 4165 | O | HOH | W | 78 | 13.365 | 25.042 | 8.721 | 1.00 | 29.68 | O |
| HETATM | 4166 | O | HOH | W | 79 | -2.835 | 16.211 | 22.213 | 1.00 | 42.69 | O |
| HETATM | 4167 | O | HOH | W | 80 | -0.806 | 13.507 | 17.668 | 1.00 | 18.89 | O |
| HETATM | 4168 | O | HOH | W | 81 | -2.772 | 7.883 | 14.041 | 1.00 | 36.25 | O |
| HETATM | 4169 | O | HOH | W | 82 | 14.336 | -0.374 | 52.681 | 1.00 | 29.69 | O |
| HETATM | 4170 | O | HOH | W | 83 | 30.767 | 13.361 | 30.094 | 1.00 | 32.30 | O |
| HETATM | 4171 | O | HOH | W | 84 | 24.728 | 15.959 | 112.079 | 1.00 | 15.48 | O |
| HETATM | 4172 | O | HOH | W | 85 | 18.585 | 5.073 | 76.156 | 1.00 | 20.77 | O |
| HETATM | 4173 | O | HOH | W | 86 | 12.087 | 6.987 | 28.731 | 1.00 | 16.34 | O |
| HETATM | 4174 | O | HOH | W | 87 | 22.672 | 3.132 | 47.075 | 1.00 | 25.24 | O |
| HETATM | 4175 | O | HOH | W | 88 | 13.707 | 29.144 | 2.429 | 1.00 | 47.19 | O |
| HETATM | 4176 | O | HOH | W | 89 | 22.063 | 15.088 | 91.588 | 1.00 | 31.79 | O |
| HETATM | 4177 | O | HOH | W | 90 | 1.459 | 6.344 | 18.792 | 1.00 | 27.32 | O |
| HETATM | 4178 | O | HOH | W | 91 | 22.534 | 16.855 | 11.275 | 1.00 | 15.54 | O |
| HETATM | 4179 | O | HOH | W | 92 | 30.290 | 7.211 | 65.189 | 1.00 | 34.30 | O |
| HETATM | 4180 | O | HOH | W | 93 | 40.141 | 30.593 | 80.818 | 1.00 | 26.41 | O |
| HETATM | 4181 | O | HOH | W | 94 | 24.536 | -1.198 | 108.080 | 1.00 | 42.66 | O |
| HETATM | 4182 | O | HOH | W | 95 | 20.853 | 15.313 | 15.256 | 1.00 | 18.03 | O |
| HETATM | 4183 | O | HOH | W | 96 | 44.683 | 13.196 | 72.750 | 1.00 | 24.69 | O |
| HETATM | 4184 | O | HOH | W | 97 | 11.740 | 1.454 | 42.593 | 1.00 | 45.99 | O |
| HETATM | 4185 | O | HOH | W | 98 | 39.581 | 13.869 | 96.751 | 1.00 | 30.88 | O |
| HETATM | 4186 | O | HOH | W | 99 | 29.670 | 2.495 | 92.023 | 1.00 | 25.37 | O |
| HETATM | 4187 | O | HOH | W | 100 | 20.178 | 12.119 | 64.978 | 1.00 | 28.53 | O |
| HETATM | 4188 | O | HOH | W | 101 | 9.026 | 2.563 | 69.045 | 1.00 | 36.54 | O |
| HETATM | 4189 | O | HOH | W | 102 | 4.213 | 30.389 | 9.007 | 1.00 | 24.44 | O |
| HETATM | 4190 | O | HOH | W | 103 | 19.707 | 24.186 | 77.524 | 1.00 | 18.74 | O |
| HETATM | 4191 | O | HOH | W | 104 | 28.504 | 18.843 | 96.342 | 1.00 | 34.10 | O |
| HETATM | 4192 | O | HOH | W | 105 | 28.044 | 9.665 | 20.495 | 1.00 | 50.29 | O |
| HETATM | 4193 | O | HOH | W | 106 | 41.926 | 5.529 | 72.212 | 1.00 | 34.69 | O |
| HETATM | 4194 | O | HOH | W | 107 | 22.321 | 10.701 | 67.907 | 1.00 | 32.90 | O |

FIG. 5RRR

| | | | | | | | | | | | |
|--------|------|---|-----|---|-----|--------|---------|--------|------|-------|---|
| HETATM | 4195 | O | HOH | W | 108 | 15.633 | 22.526 | 83.643 | 1.00 | 23.10 | O |
| HETATM | 4196 | O | HOH | W | 109 | 23.131 | 15.975 | 74.461 | 1.00 | 21.55 | O |
| HETATM | 4197 | O | HOH | W | 110 | 20.206 | -1.361 | 3.237 | 1.00 | 24.94 | O |
| HETATM | 4198 | O | HOH | W | 111 | 25.315 | 4.505 | 14.304 | 1.00 | 25.25 | O |
| HETATM | 4199 | O | HOH | W | 112 | 11.883 | 15.625 | 28.119 | 1.00 | 39.37 | O |
| HETATM | 4200 | O | HOH | W | 113 | 18.166 | 32.386 | 17.278 | 1.00 | 24.17 | O |
| HETATM | 4201 | O | HOH | W | 114 | -2.720 | 14.293 | 24.689 | 1.00 | 30.63 | O |
| HETATM | 4202 | O | HOH | W | 115 | 37.824 | 15.970 | 60.577 | 1.00 | 33.16 | O |
| HETATM | 4203 | O | HOH | W | 116 | 48.148 | 29.585 | 73.317 | 1.00 | 29.82 | O |
| HETATM | 4204 | O | HOH | W | 117 | 27.520 | 13.412 | 42.579 | 1.00 | 31.21 | O |
| HETATM | 4205 | O | HOH | W | 118 | 15.247 | 11.867 | 76.998 | 1.00 | 18.28 | O |
| HETATM | 4206 | O | HOH | W | 119 | 40.508 | 24.823 | 69.040 | 1.00 | 22.36 | O |
| HETATM | 4207 | O | HOH | W | 120 | 30.616 | 39.569 | 77.139 | 1.00 | 37.78 | O |
| HETATM | 4208 | O | HOH | W | 121 | 24.291 | 11.180 | 25.560 | 1.00 | 30.20 | O |
| HETATM | 4209 | O | HOH | W | 122 | 4.042 | 25.207 | 20.826 | 1.00 | 22.39 | O |
| HETATM | 4210 | O | HOH | W | 123 | 29.792 | 14.975 | 63.464 | 1.00 | 26.82 | O |
| HETATM | 4211 | O | HOH | W | 124 | 21.491 | 3.300 | 43.251 | 1.00 | 29.55 | O |
| HETATM | 4212 | O | HOH | W | 125 | -2.406 | 5.673 | 5.899 | 1.00 | 40.95 | O |
| HETATM | 4213 | O | HOH | W | 126 | 41.952 | 0.853 | 64.026 | 1.00 | 39.40 | O |
| HETATM | 4214 | O | HOH | W | 127 | 26.223 | 32.496 | 71.464 | 1.00 | 20.59 | O |
| HETATM | 4215 | O | HOH | W | 128 | 41.042 | 17.410 | 89.676 | 1.00 | 22.01 | O |
| HETATM | 4216 | O | HOH | W | 129 | 16.372 | 13.385 | 48.181 | 1.00 | 26.56 | O |
| HETATM | 4217 | O | HOH | W | 130 | 11.751 | -0.808 | 7.821 | 1.00 | 34.38 | O |
| HETATM | 4218 | O | HOH | W | 131 | 16.558 | 15.676 | 34.571 | 1.00 | 27.55 | O |
| HETATM | 4219 | O | HOH | W | 132 | 23.715 | -1.482 | 0.235 | 1.00 | 25.41 | O |
| HETATM | 4220 | O | HOH | W | 133 | 26.293 | 12.543 | 37.315 | 1.00 | 31.89 | O |
| HETATM | 4221 | O | HOH | W | 134 | 14.899 | 3.023 | -3.088 | 1.00 | 34.89 | O |
| HETATM | 4222 | O | HOH | W | 135 | 26.593 | -11.074 | 49.839 | 1.00 | 39.76 | O |
| HETATM | 4223 | O | HOH | W | 136 | 15.743 | 30.206 | 24.249 | 1.00 | 31.35 | O |
| HETATM | 4224 | O | HOH | W | 137 | 42.127 | 14.189 | 92.996 | 1.00 | 31.84 | O |
| HETATM | 4225 | O | HOH | W | 138 | 29.099 | 8.319 | 61.777 | 1.00 | 34.30 | O |
| HETATM | 4226 | O | HOH | W | 139 | 17.387 | 15.237 | 55.947 | 1.00 | 37.57 | O |
| HETATM | 4227 | O | HOH | W | 140 | 39.225 | 28.436 | 85.846 | 1.00 | 37.70 | O |
| HETATM | 4228 | O | HOH | W | 141 | 18.972 | 32.465 | 70.632 | 1.00 | 35.06 | O |
| HETATM | 4229 | O | HOH | W | 142 | 17.480 | 17.370 | 27.959 | 1.00 | 42.72 | O |
| HETATM | 4230 | O | HOH | W | 143 | 17.684 | 35.863 | 15.728 | 1.00 | 40.59 | O |
| HETATM | 4231 | O | HOH | W | 144 | 33.135 | 22.579 | 69.723 | 1.00 | 34.19 | O |
| HETATM | 4232 | O | HOH | W | 145 | 19.206 | 21.593 | 75.835 | 1.00 | 39.22 | O |
| HETATM | 4233 | O | HOH | W | 146 | 22.243 | 7.202 | 91.152 | 1.00 | 38.82 | O |
| HETATM | 4234 | O | HOH | W | 147 | 24.911 | 14.181 | 43.275 | 1.00 | 41.58 | O |
| HETATM | 4235 | O | HOH | W | 148 | 22.856 | -12.981 | 28.140 | 1.00 | 39.84 | O |
| HETATM | 4236 | O | HOH | W | 149 | 22.202 | -8.821 | 40.526 | 1.00 | 40.27 | O |
| HETATM | 4237 | O | HOH | W | 150 | 21.291 | 37.012 | 72.400 | 1.00 | 43.51 | O |
| HETATM | 4238 | O | HOH | W | 151 | 22.094 | -11.920 | 56.697 | 1.00 | 36.84 | O |
| HETATM | 4239 | O | HOH | W | 152 | 13.637 | 16.495 | 29.478 | 1.00 | 40.50 | O |
| HETATM | 4240 | O | HOH | W | 153 | 21.255 | 21.183 | 48.853 | 1.00 | 42.81 | O |
| HETATM | 4241 | O | HOH | W | 154 | 41.602 | 15.939 | 96.547 | 1.00 | 34.07 | O |
| HETATM | 4242 | O | HOH | W | 155 | 23.933 | 13.479 | 26.357 | 1.00 | 43.11 | O |
| HETATM | 4243 | O | HOH | W | 156 | 18.066 | 2.265 | -8.683 | 1.00 | 41.94 | O |
| HETATM | 4244 | O | HOH | W | 157 | 1.561 | 20.646 | 25.469 | 1.00 | 41.00 | O |
| HETATM | 4245 | O | HOH | W | 158 | 25.489 | 32.498 | 17.399 | 1.00 | 36.46 | O |
| HETATM | 4246 | O | HOH | W | 159 | 14.812 | -6.860 | 22.670 | 1.00 | 36.94 | O |
| HETATM | 4247 | O | HOH | W | 160 | 16.597 | 18.943 | 19.645 | 1.00 | 34.23 | O |
| HETATM | 4248 | O | HOH | W | 161 | 17.808 | 4.769 | 51.095 | 1.00 | 41.29 | O |
| END | | | | | | | | | | | |

FIG. 5SSS

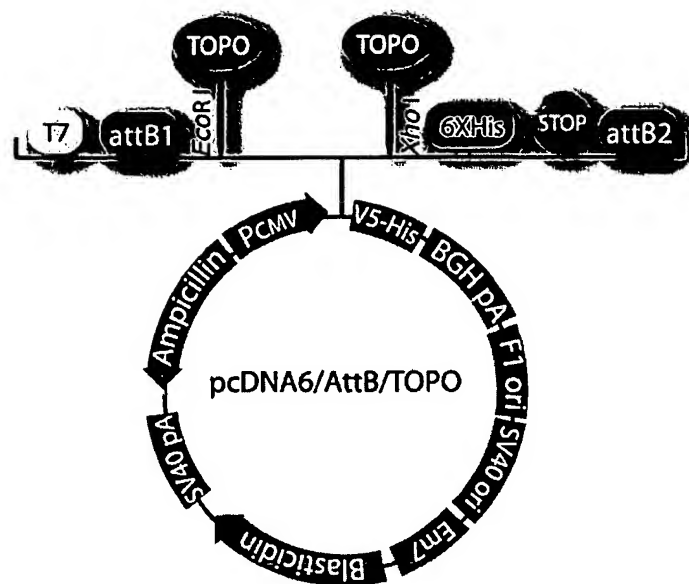


FIG. 6

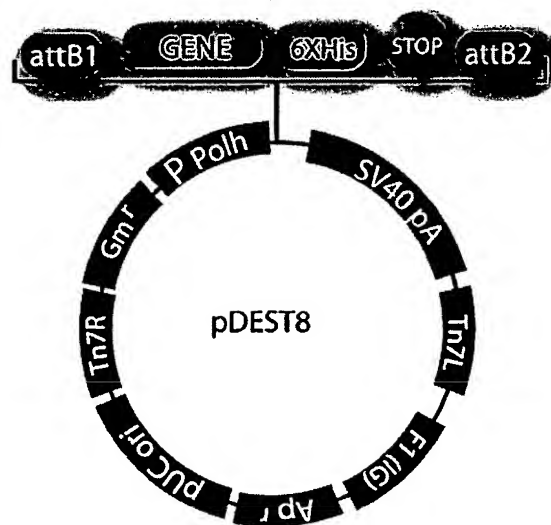


FIG. 7